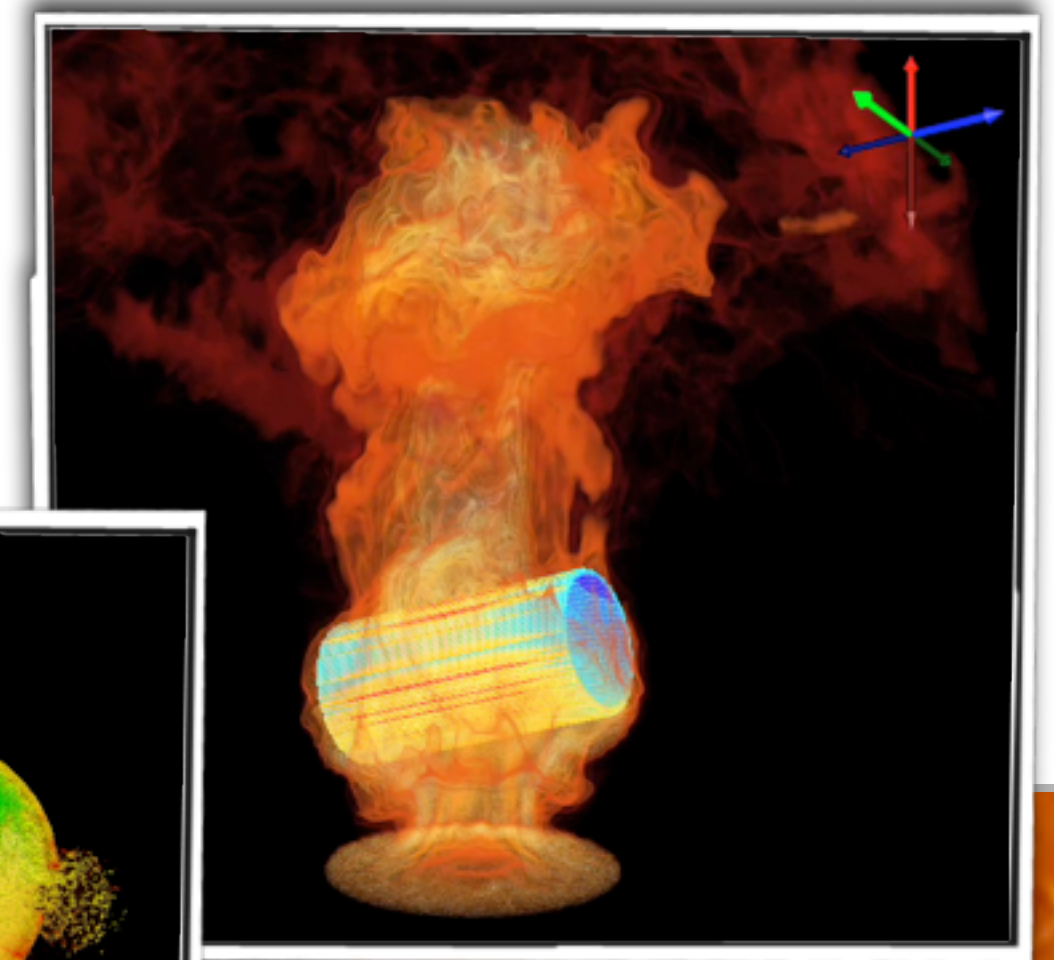
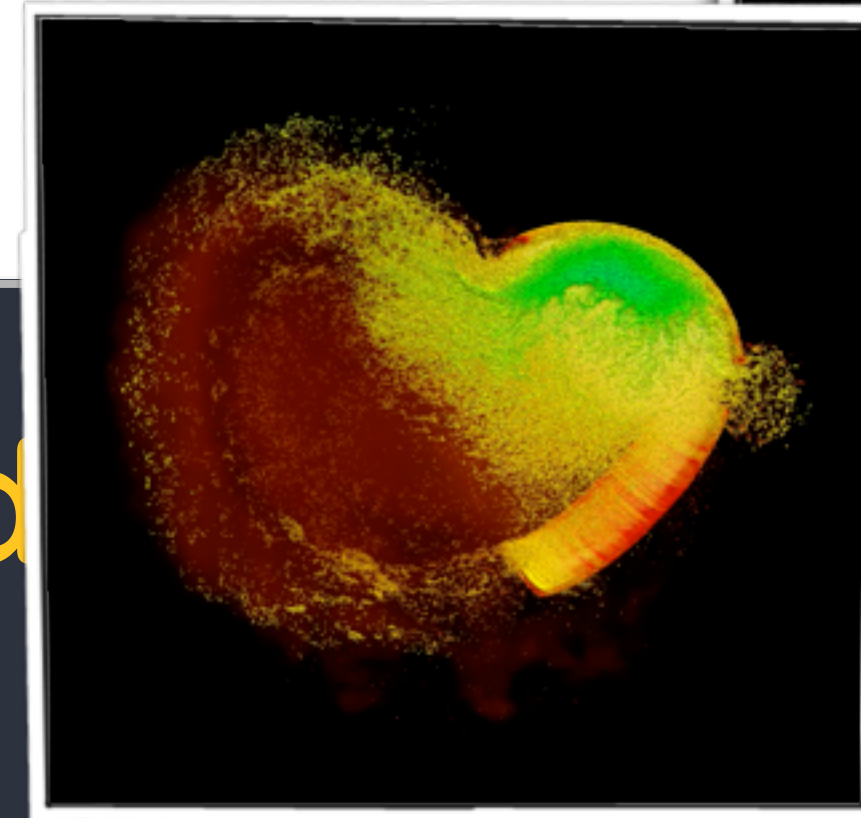




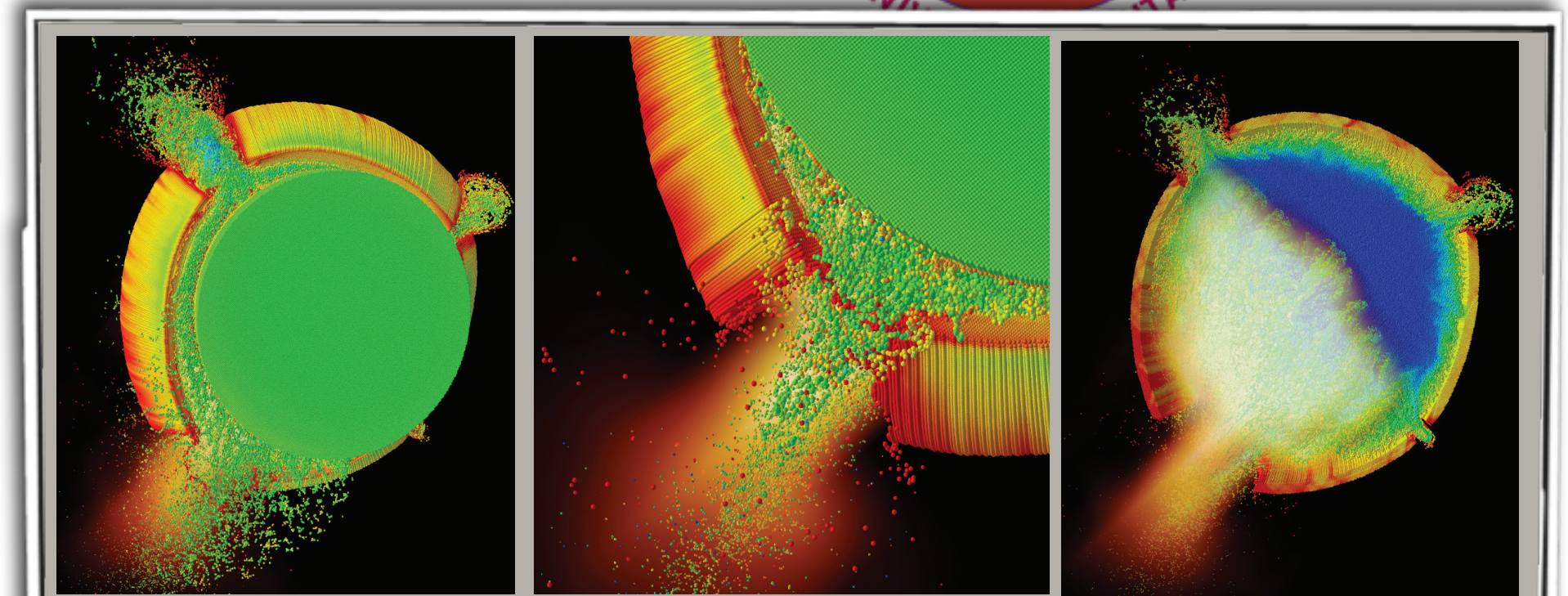
Center for Simulation of Accidental Fires & Explosions



Center for Simulation of Accidents Fires & Explosions

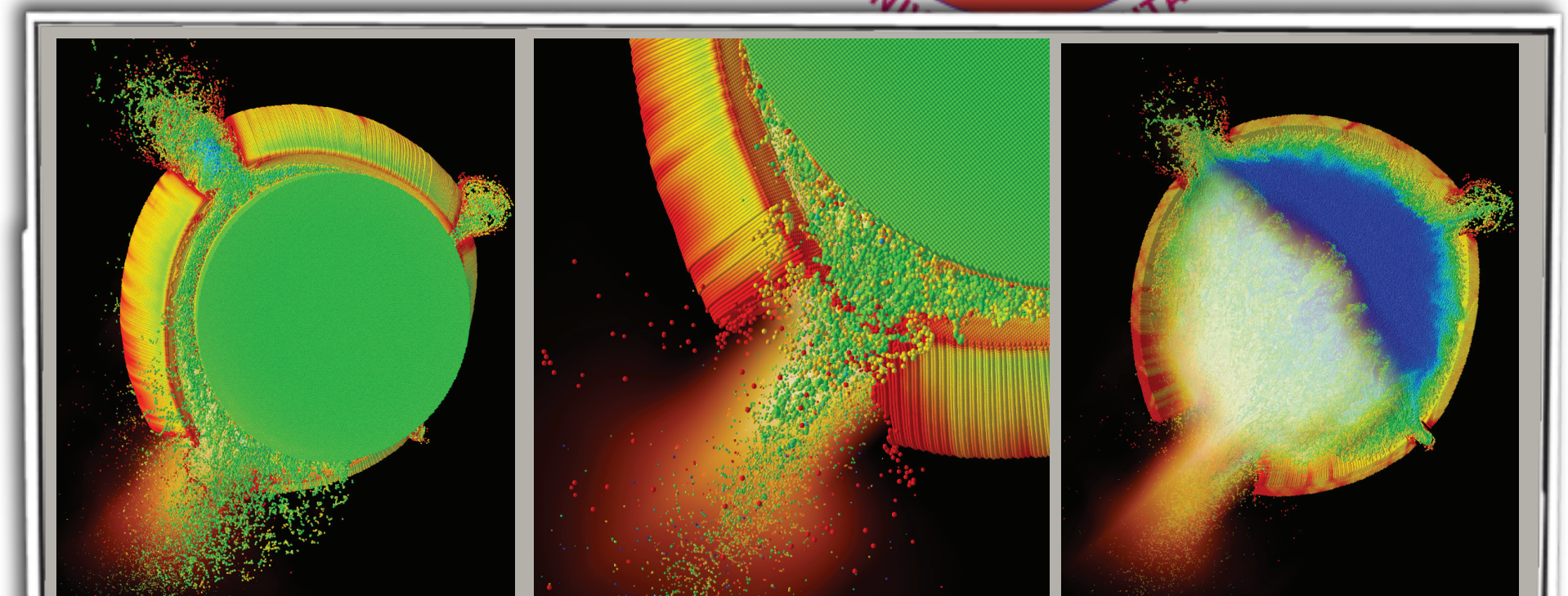
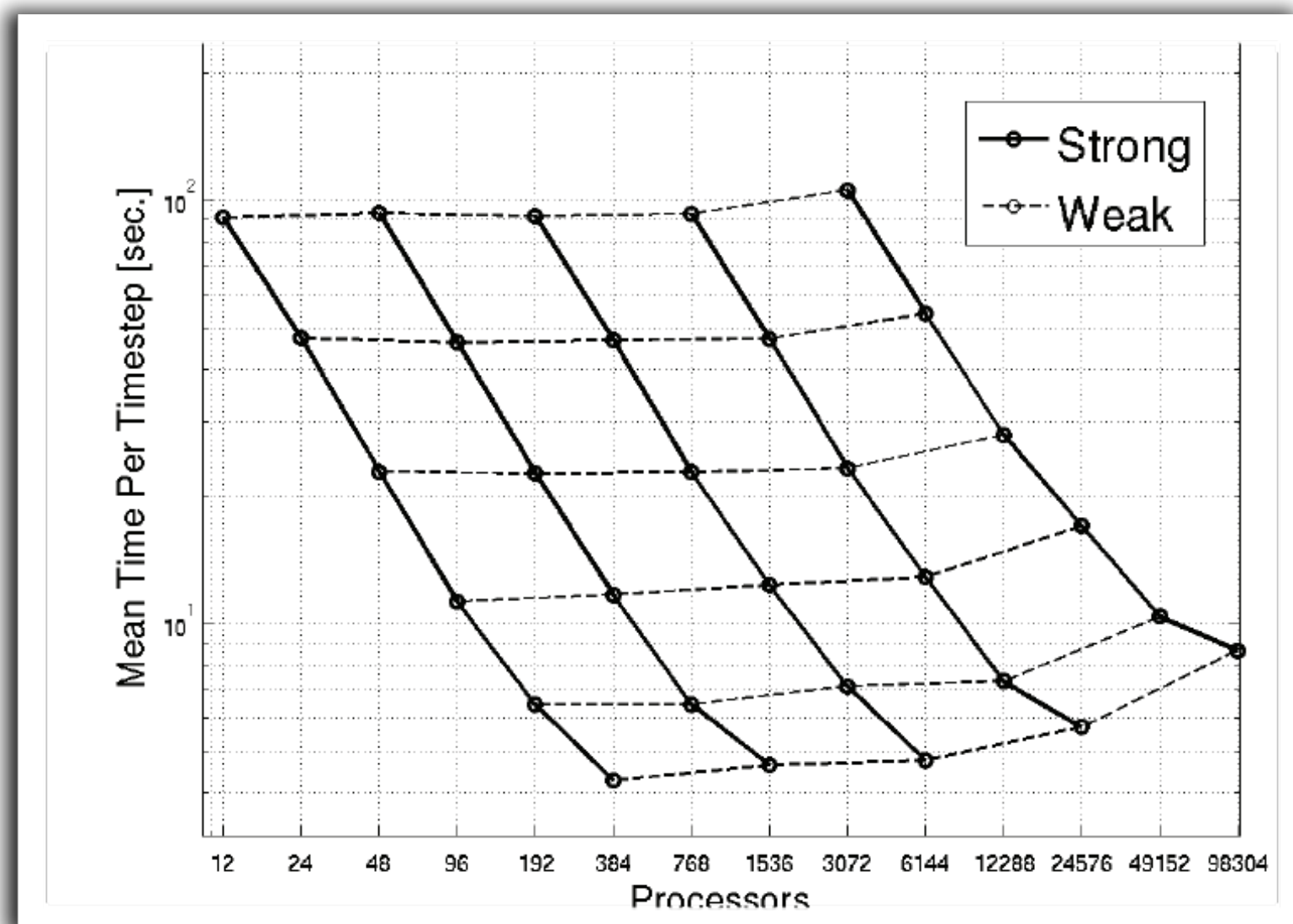
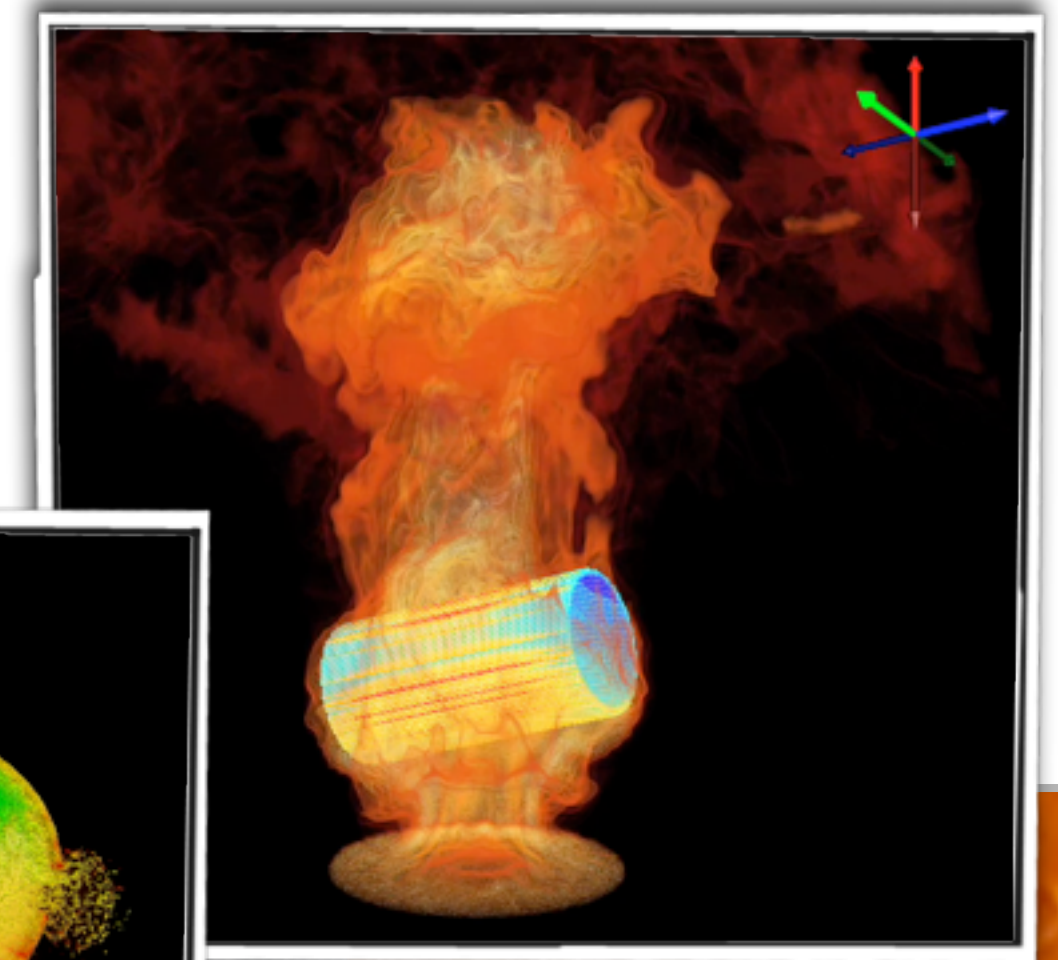
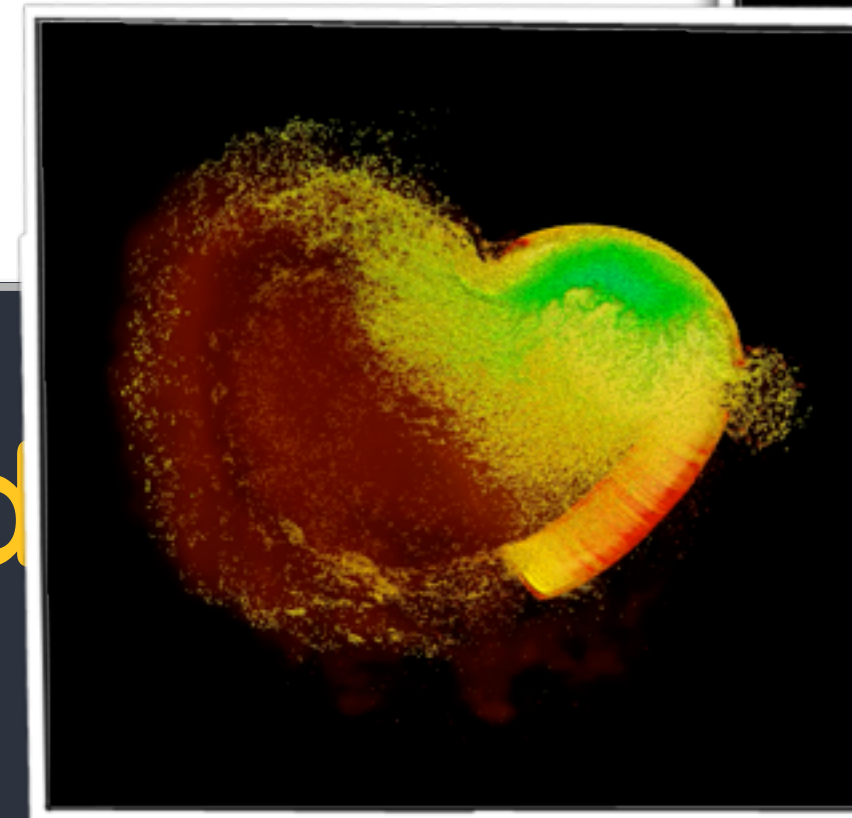


- Untah Computational Framework**
component based software system
- semi-automatic parallelism
 - checkpoint/restart
 - load-balancing / scheduling
 - execution model
 - task graph: computations expressed as directed acyclic graphs of tasks
 - load balancing is done by using a fast space filling curve algorithm



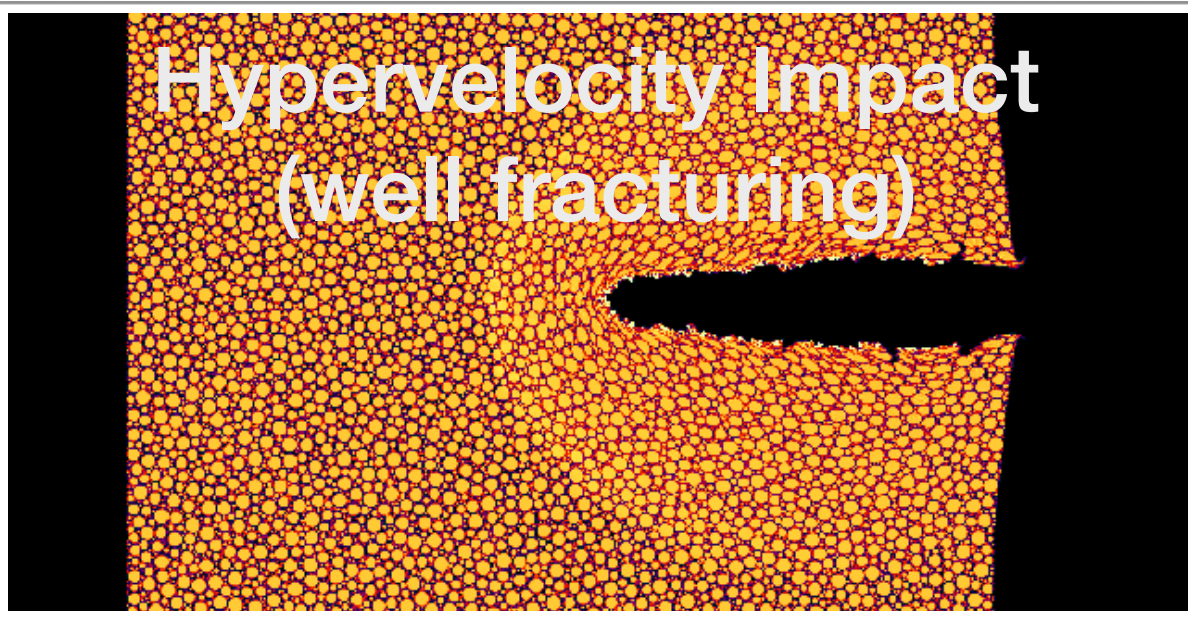
This coupled multi-physics integrated simulation consists of three phases (all run within the UCF). First is the simulation of the fire and calculates the time averaged rate of heat transfer to the container. Second is the heat up of the container in which the heat is transferred from the fire, through the container, and into the explosive. The final phase occurs when the explosive begins to convert from the solid to the gaseous phase.

Center for Simulation of Accidents Fires & Explosions



This coupled multi-physics integrated simulation consists of three phases (all run within the UCF). First is the simulation of the fire and calculates the time averaged rate of heat transfer to the container. Second is the heat up of the container in which the heat is transferred from the fire, through the container, and into the explosive. The final phase occurs when the explosive begins to convert from the solid to the gaseous phase.

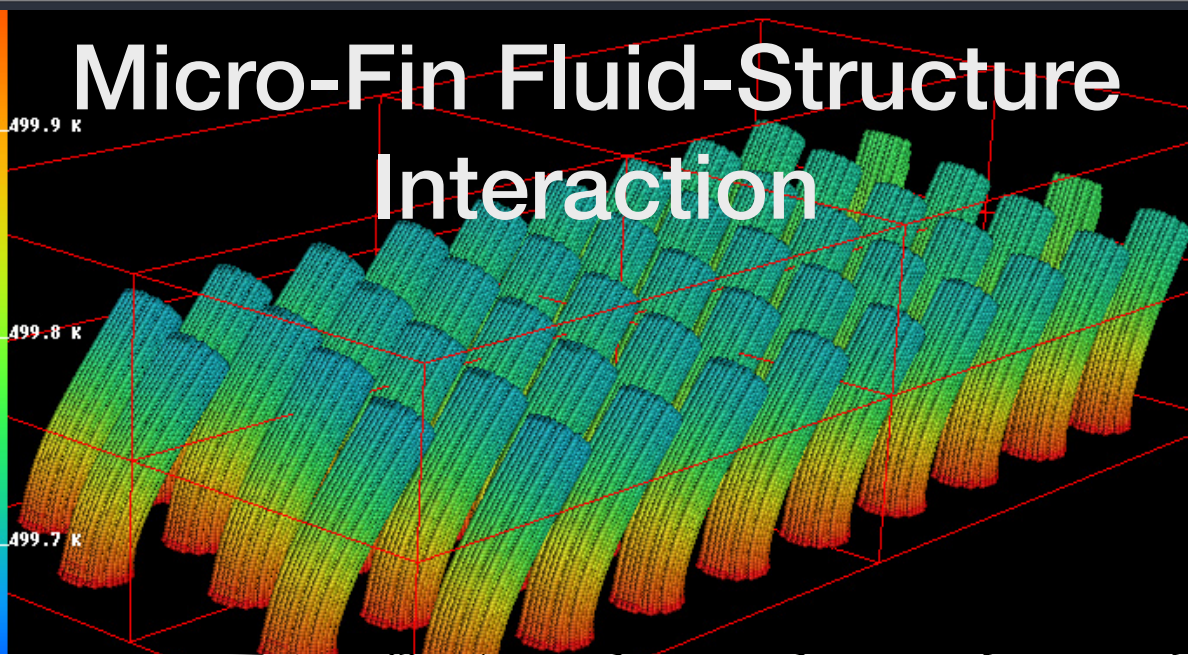
Hypervelocity Impact
(well fracturing)



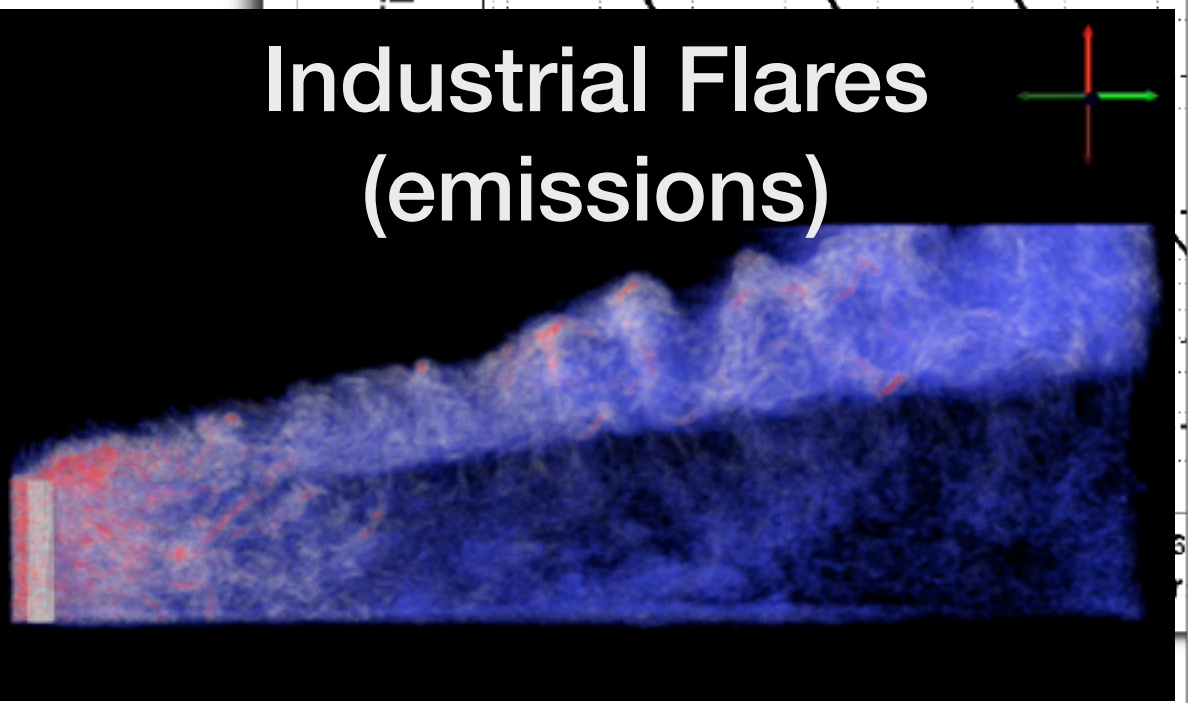
Coal-Fired Burners
(ignition)



Micro-Fin Fluid-Structure
Interaction

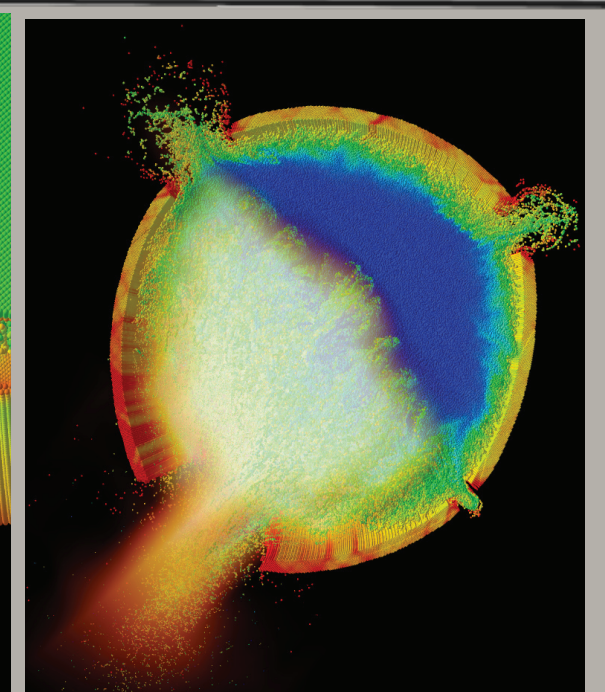
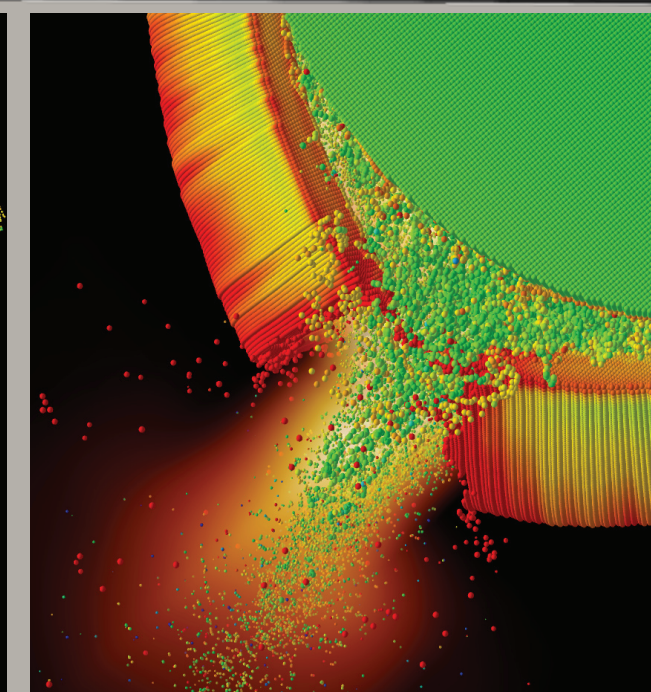
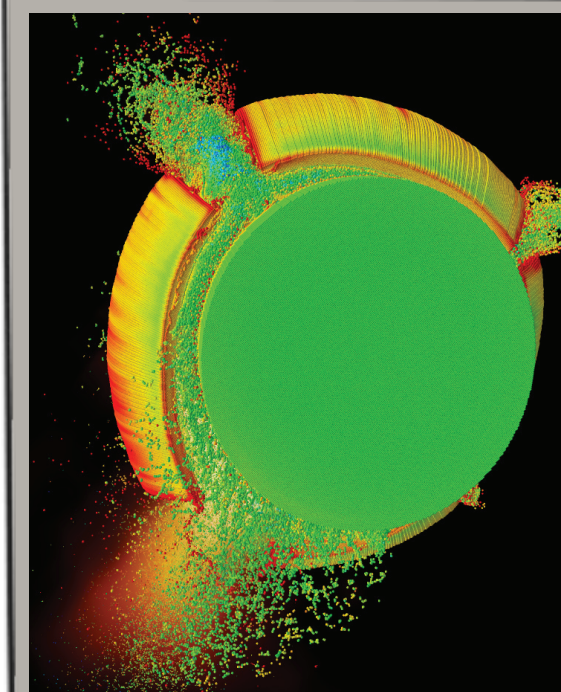
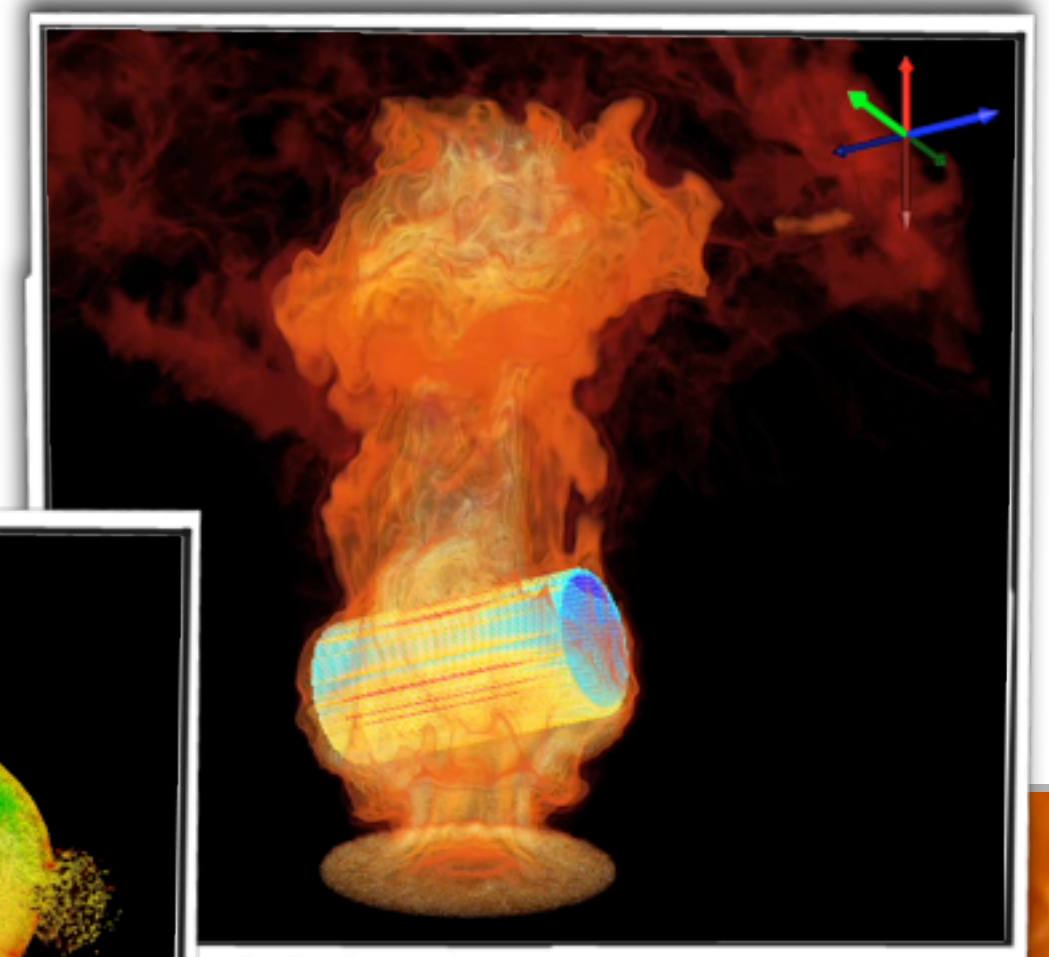
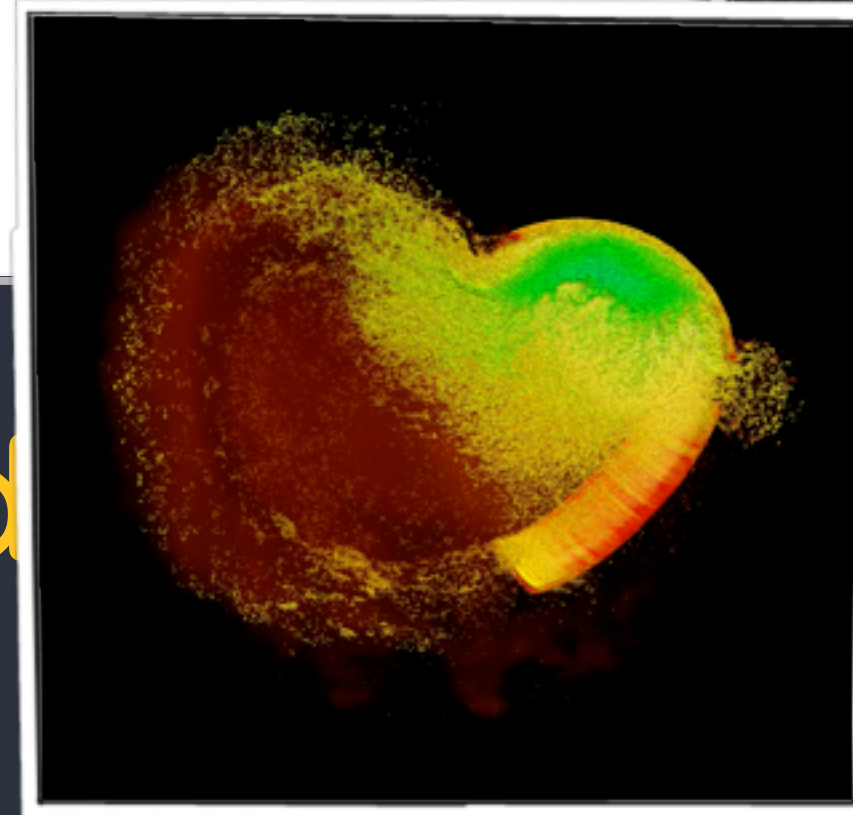


Industrial Flares
(emissions)

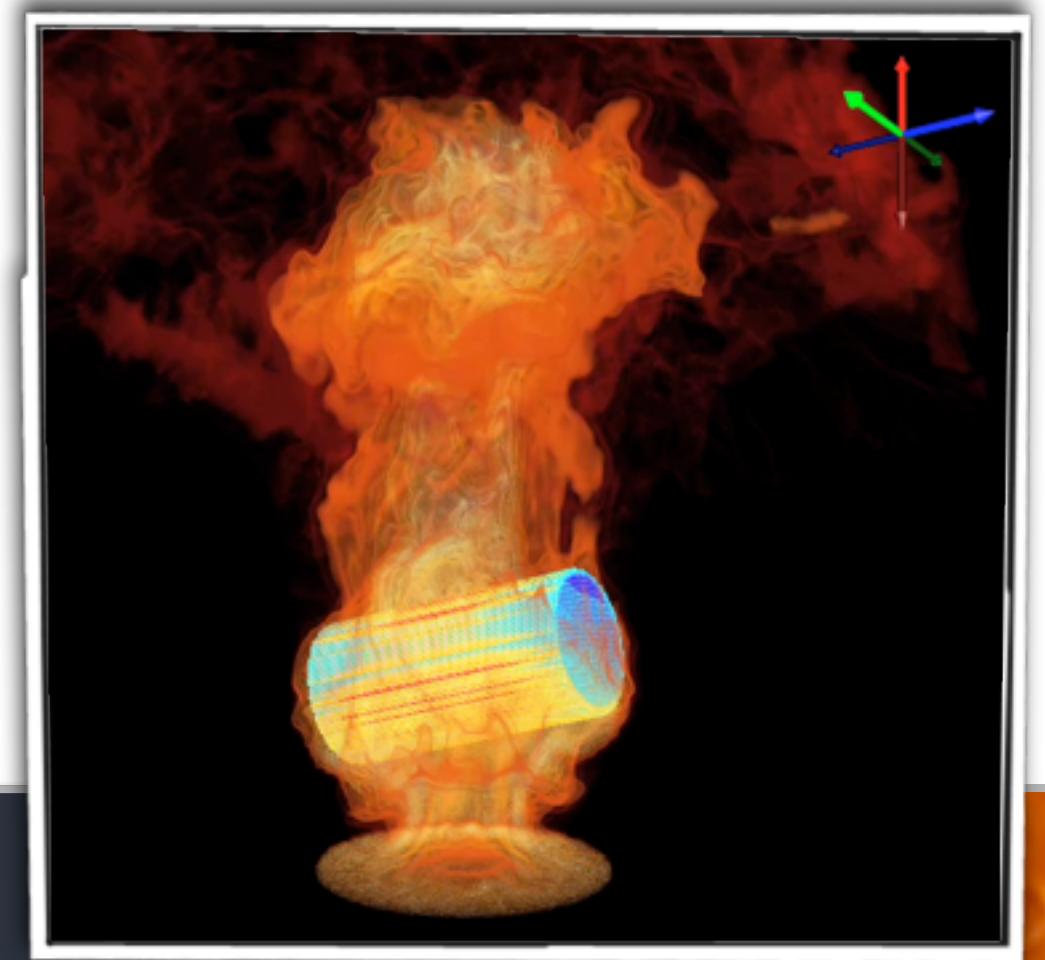


UNIVERSITY OF UTAH®

Simulation of Accidents
Explosions



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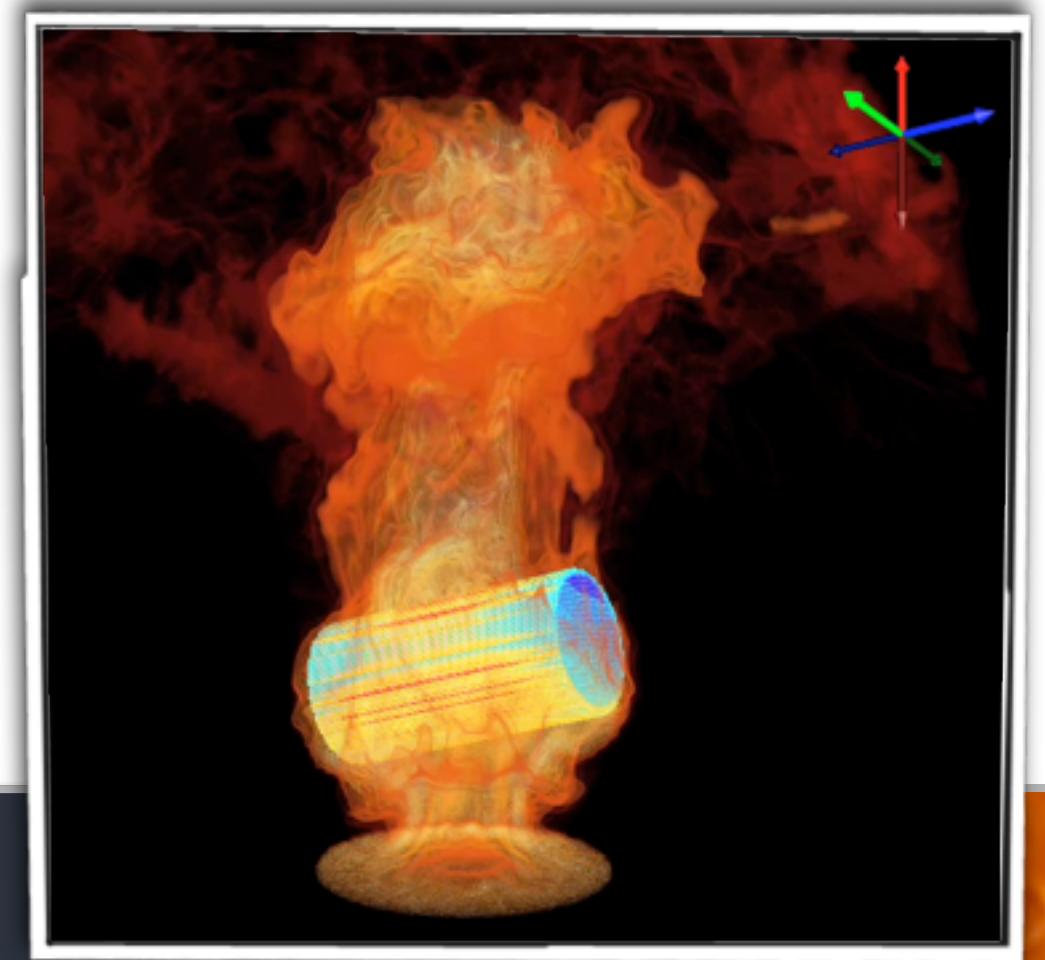
Validation / Uncertainty Quantification *integrating experiments & simulations*



validation:

$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$

source of uncertainty?



Validation / Uncertainty Quantification *integrating experiments & simulations*

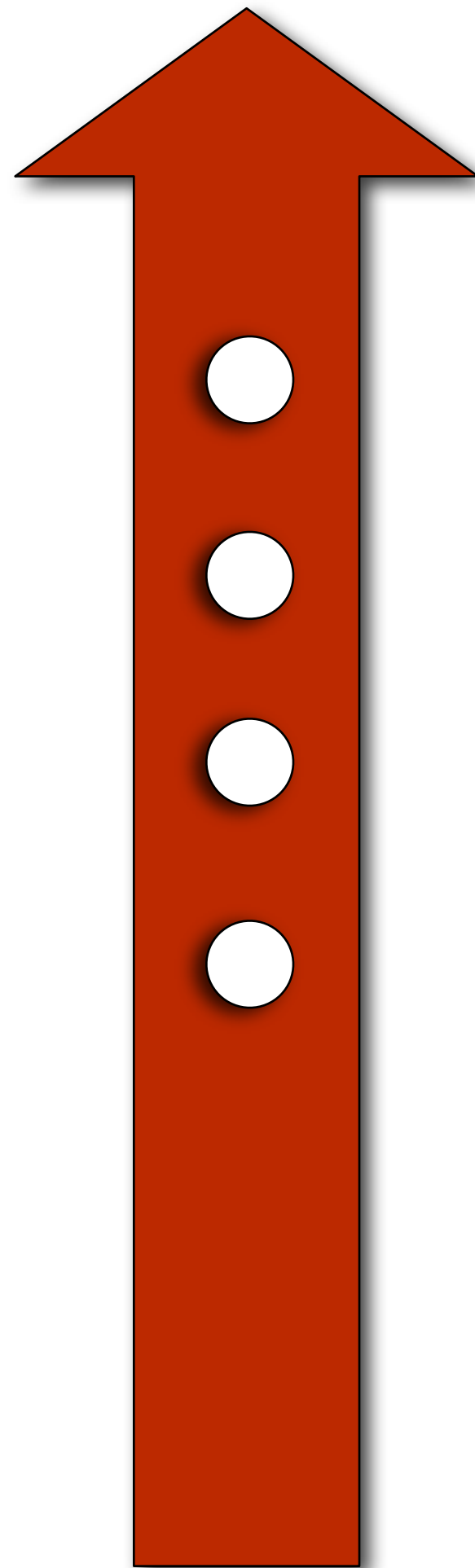


prediction:

$$\left| y_m(x) - \cancel{y_{\text{exp}}} \right| \leq u$$

?

$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$



Experimental Uncertainty ($y_e \pm u_e$)

Verification Error - Numerics ($y_v \pm u_v$)

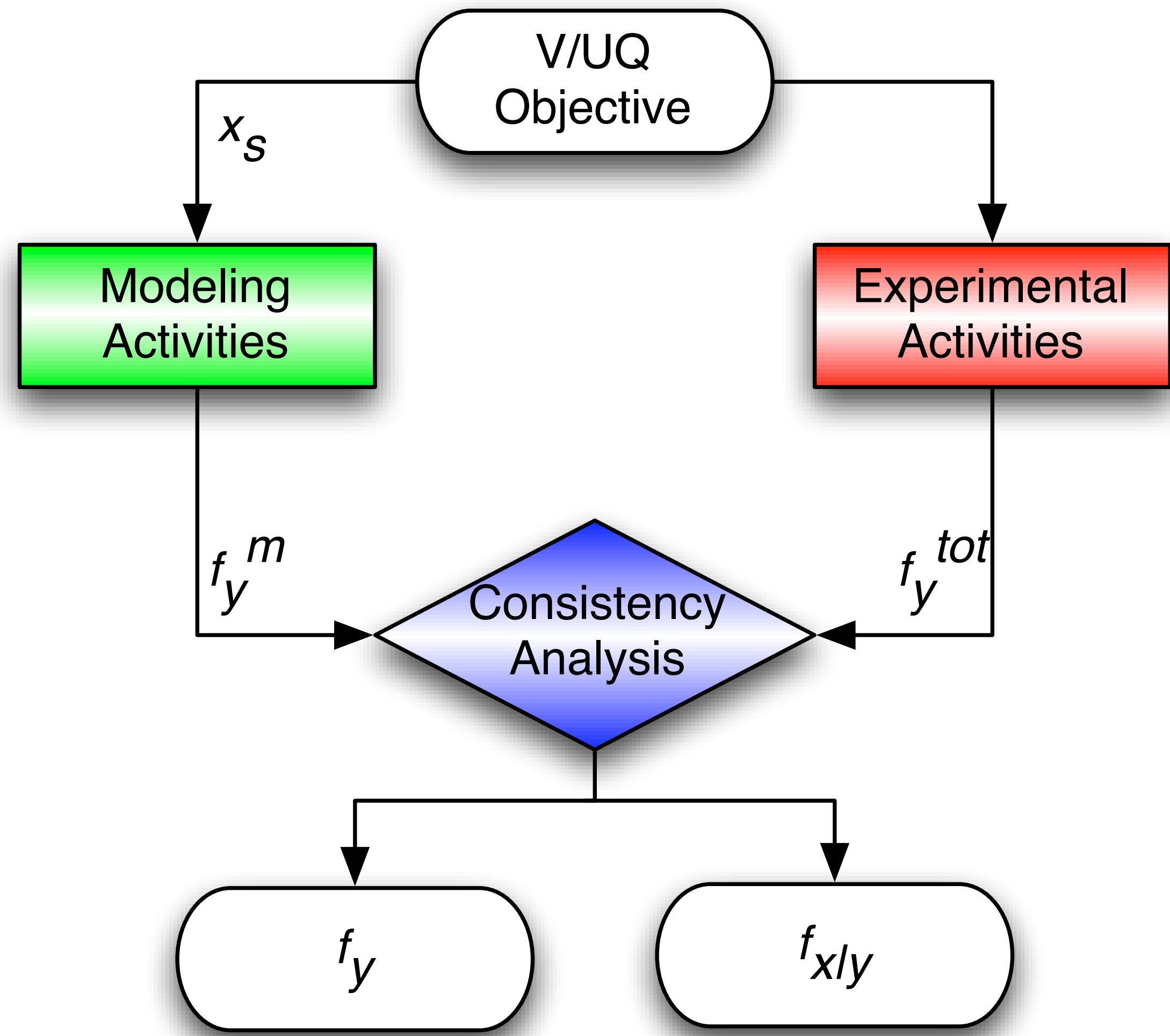
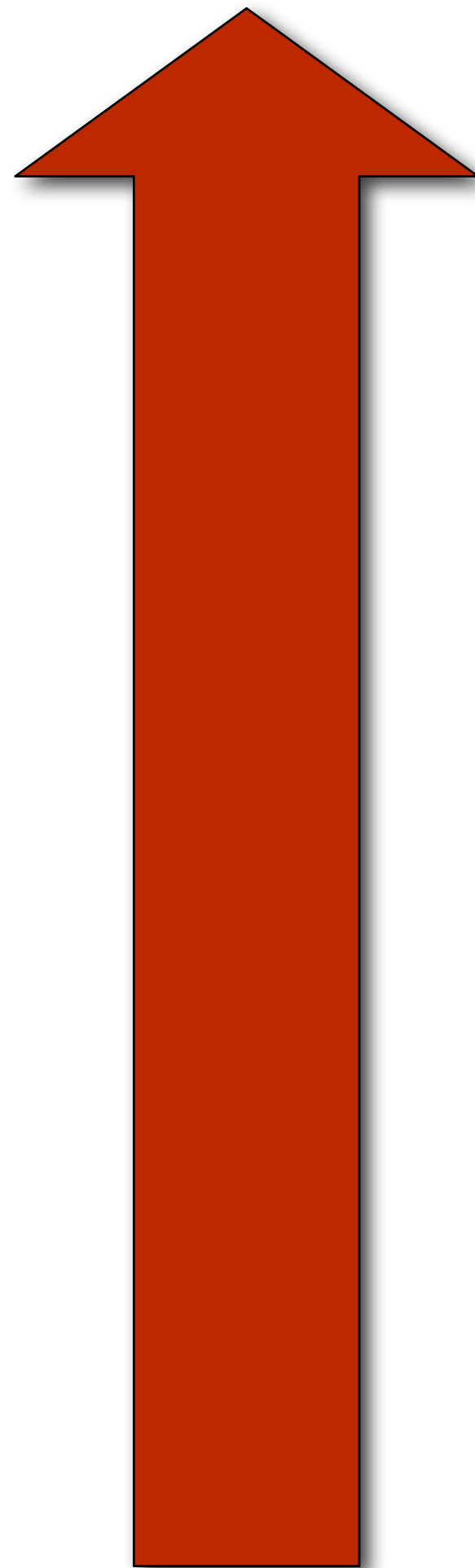
Models / Model Parameters ($x_m \pm u_m$)

Scenario Parameters ($x_s \pm u_s$)

Error Budget: validation/uncertainty quantification



$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$



Error Budget: validation/uncertainty quantification



$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$

Consistency*
= maximum
value of γ
subject to
constraints

$$\left\{ \begin{array}{l} -x_j \leq -\alpha_j \\ x_j \leq \beta_j \\ -y_m(\mathbf{x}_e) + y_e \leq l_e - \gamma \\ y_m(\mathbf{x}_e) - y_e \leq u_e - \gamma \end{array} \right.$$

*see Feeley et al. *J. Phys. Chem. A* 2004, 108, 9573-9583

$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$

- **V/UQ algorithm:**

- from prior knowledge identify estimate of uncertainty bounds (hierarchical validation analysis)
- build surrogate model spanning uncertainty space
- estimate experimental uncertainty bounds
- identify consistent bounds (validation)
- predict new scenario (prediction)

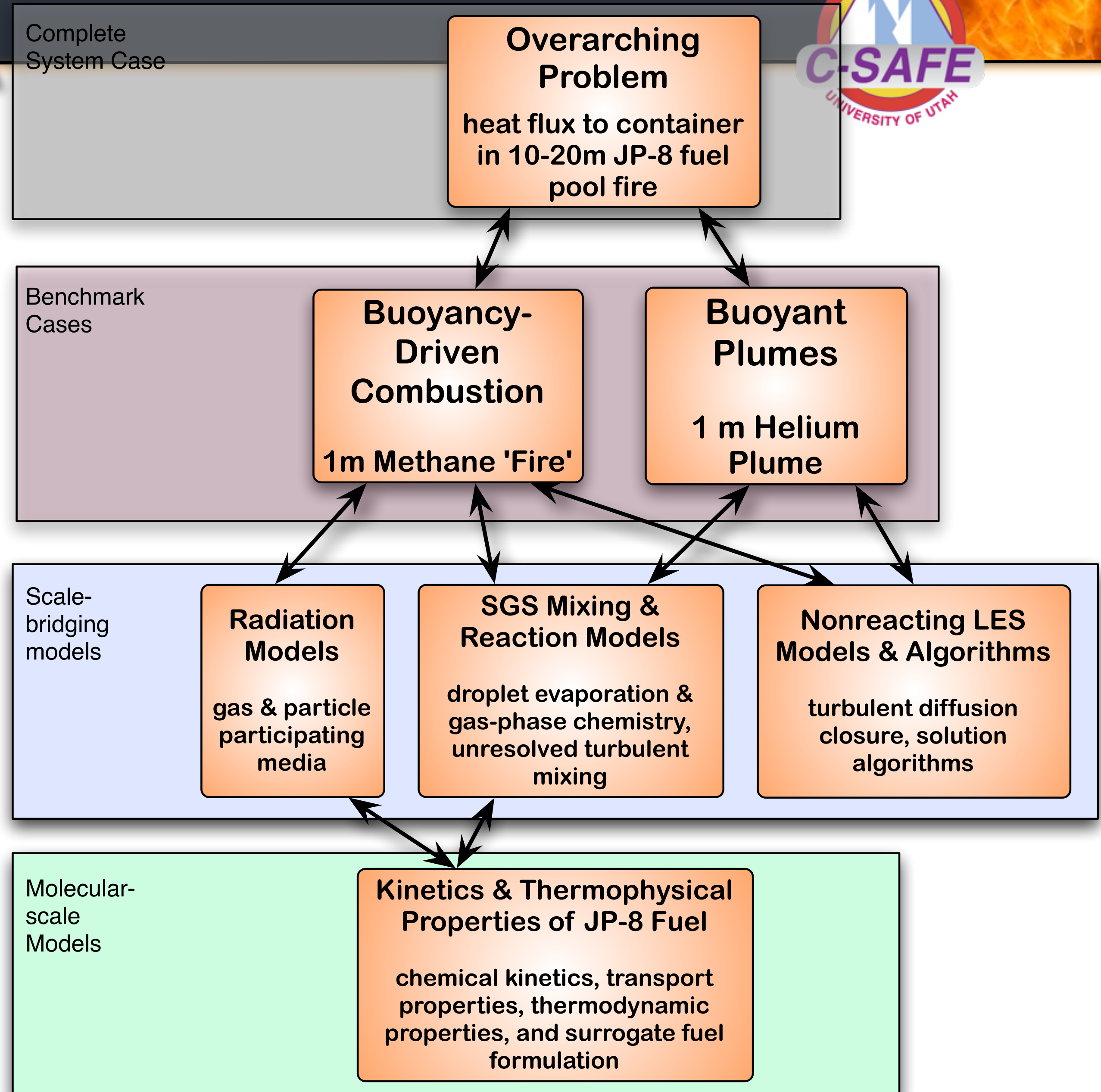
-
- integration of scales & physics
 - integration of simulation & experiments
 - high performance computing

Hierarchical V/UQ

scalable
multi-scale
multi-physics

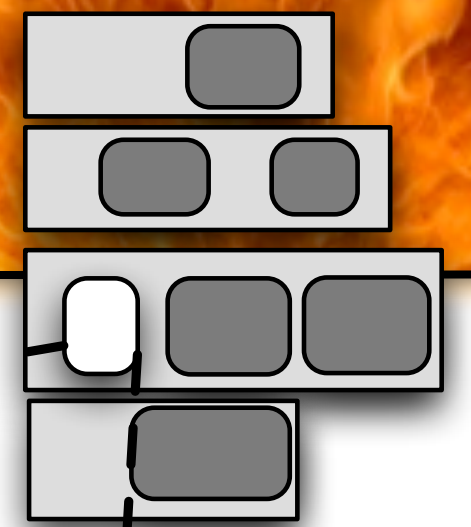
sparse data

expensive function evaluations

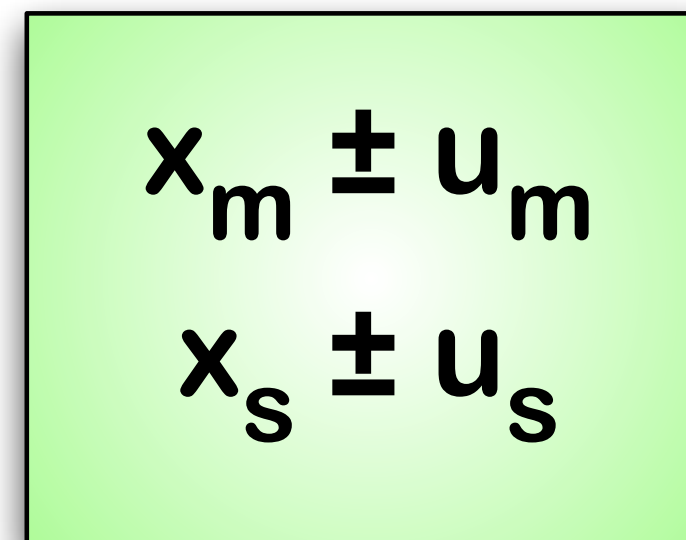


Hierarchical V/UQ

scalable
multi-scale
multi-physics



Priors



**Bridging
Model**
 $y_m(x)$

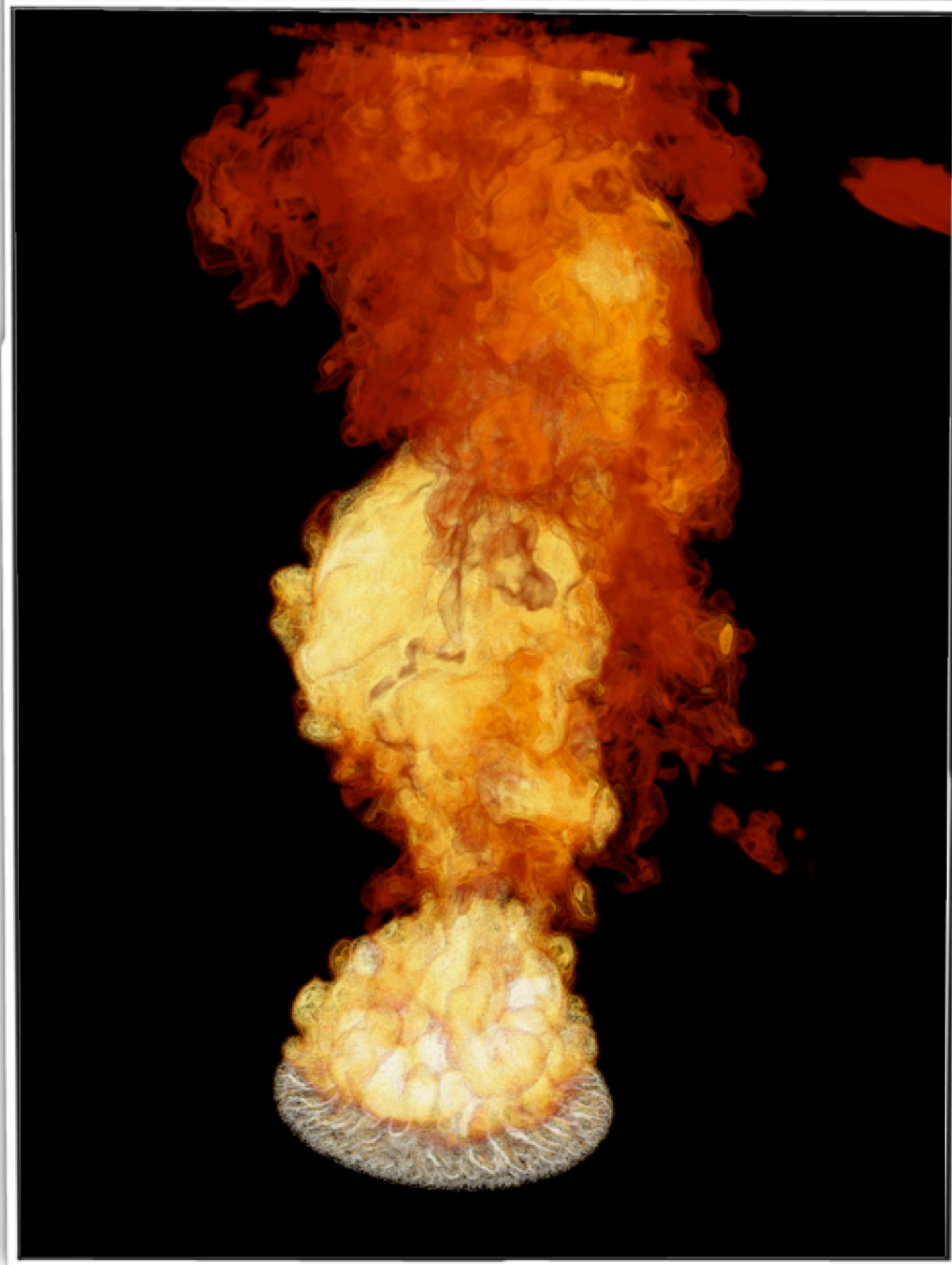
Posterior

Output
 $y_m \pm u_m$
 $x_m \pm u_m$
 $x_s \pm u_s$

Experimental Data ($y \pm u_v$)

Buoyant Plumes

$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$



Complete
System Case

**Overarching
Problem**

heat flux to container
in 10-20m JP-8 fuel
pool fire



Benchmark
Cases

**Buoyancy-
Driven
Combustion**

1m Methane 'Fire'

**Buoyant
Plumes**

1 m Helium
Plume

Scale-
bridging
models

**Radiation
Models**

gas & particle
participating
media

**SGS Mixing &
Reaction Models**

droplet evaporation &
gas-phase chemistry,
unresolved turbulent
mixing

**Nonreacting LES
Models & Algorithms**

turbulent diffusion
closure, solution
algorithms

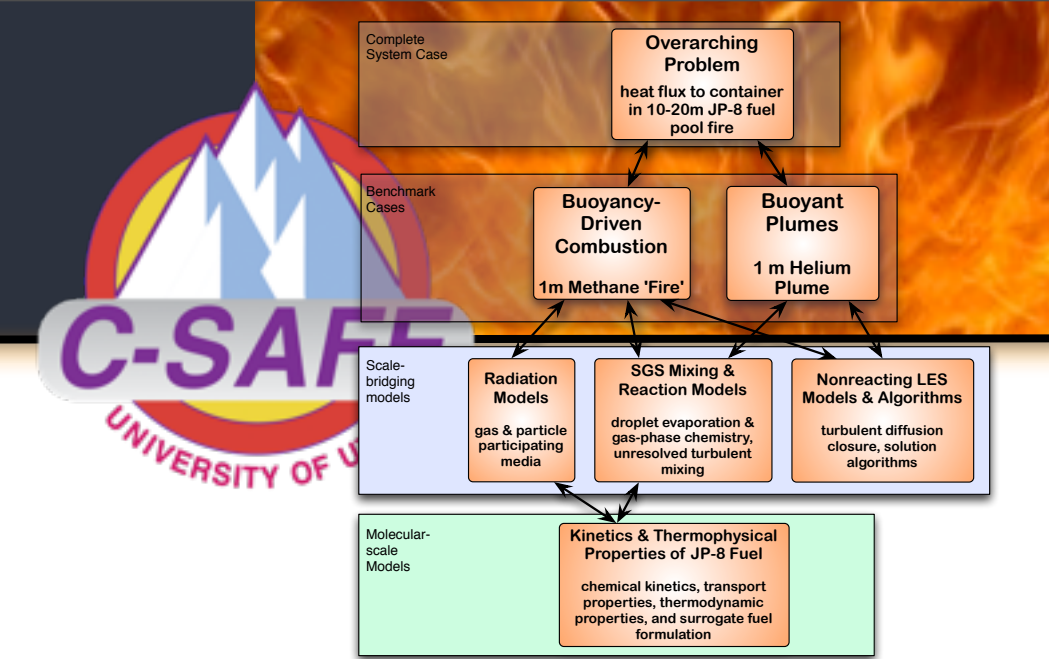
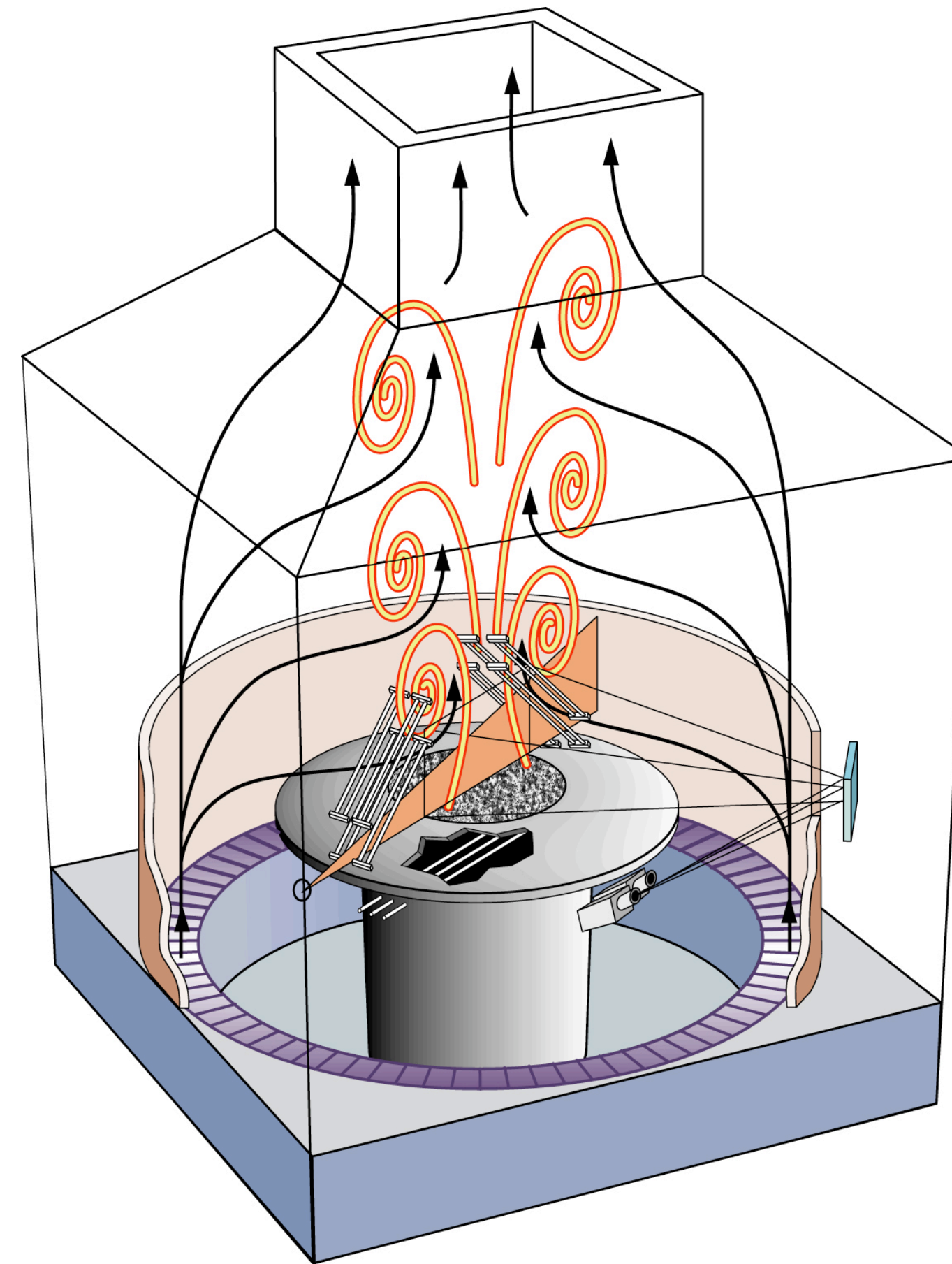
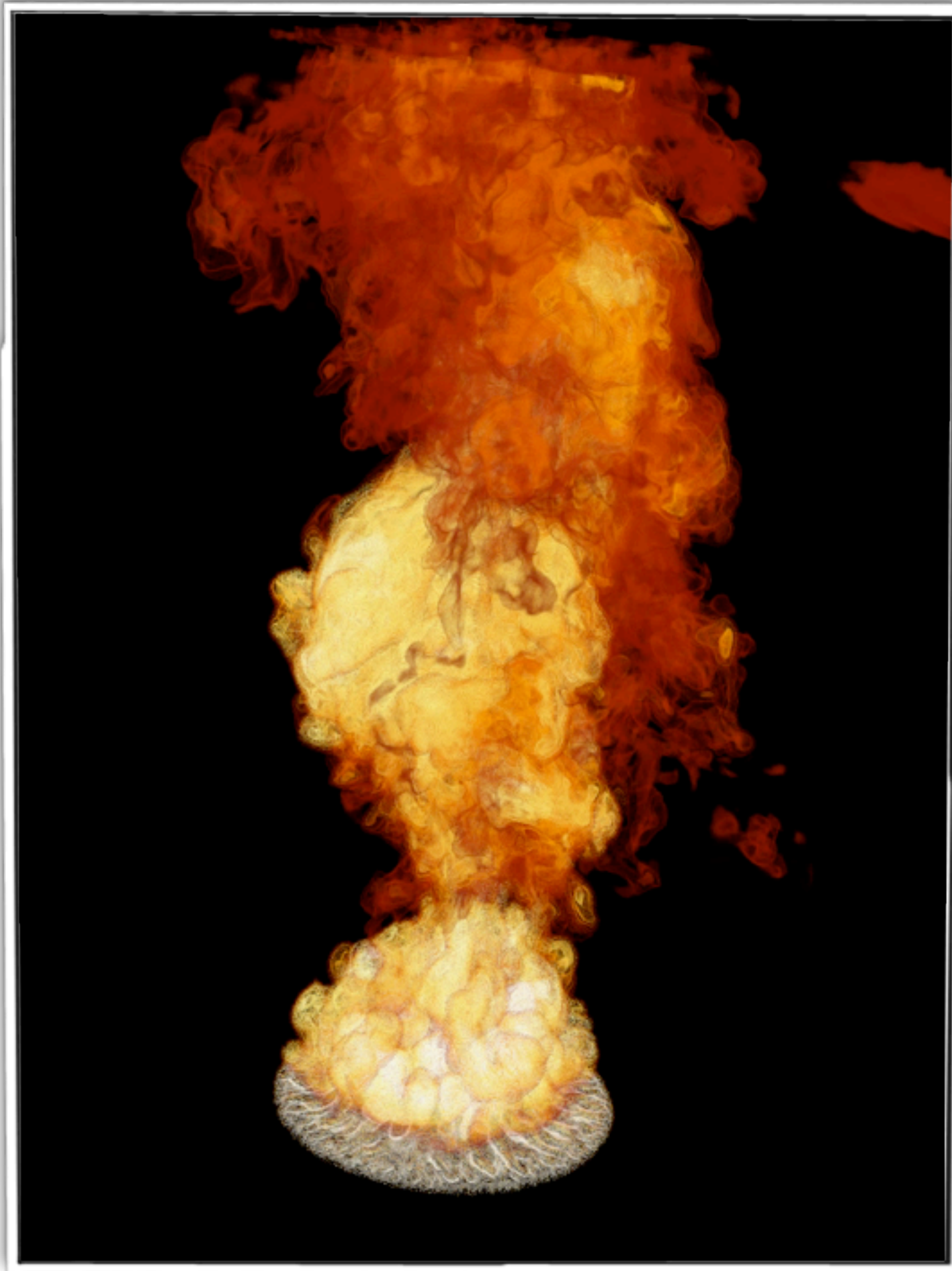
Molecular-
scale
Models

**Kinetics & Thermophysical
Properties of JP-8 Fuel**

chemical kinetics, transport
properties, thermodynamic
properties, and surrogate fuel
formulation

Buoyant Plumes

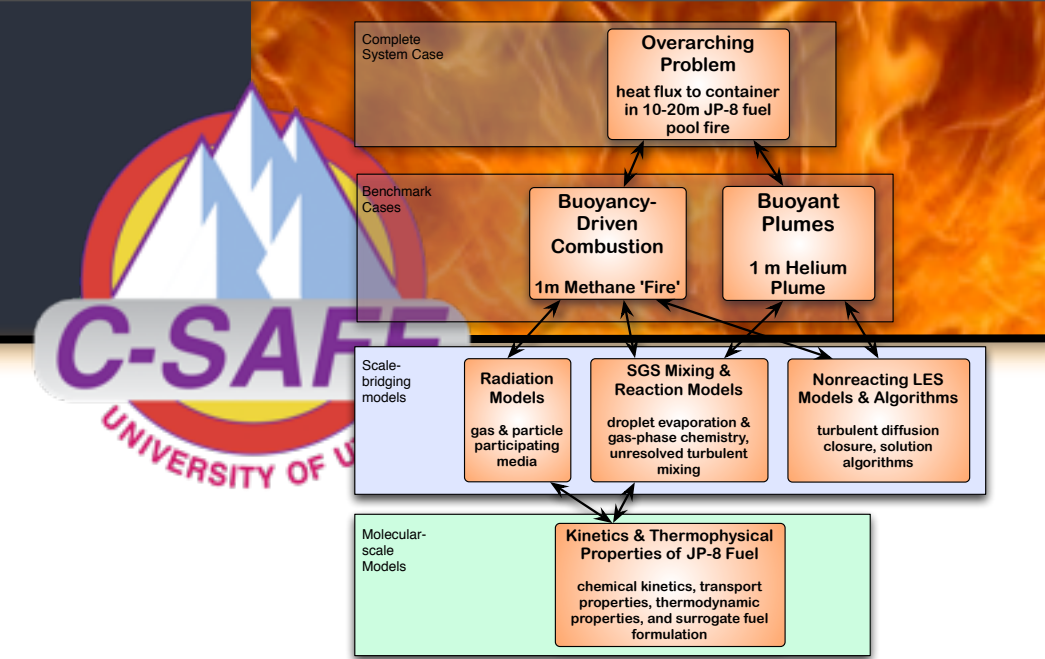
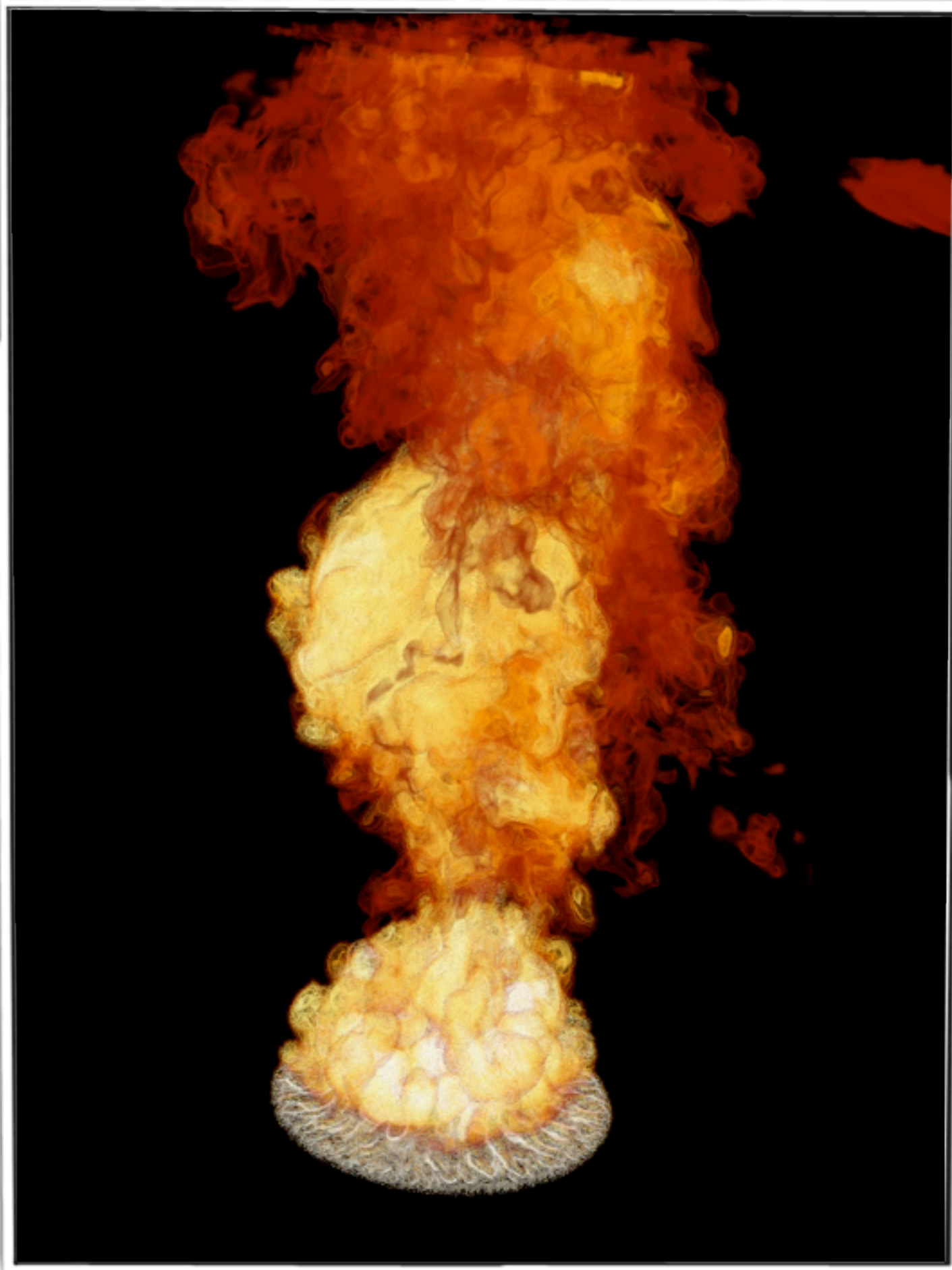
$$\left| y_m(x) - y_{\text{exp}} \right| \leq u$$



experiments from Sandia FLAME facility - Tieszen et al. (Sandia National Laboratory)

Buoyant Plumes

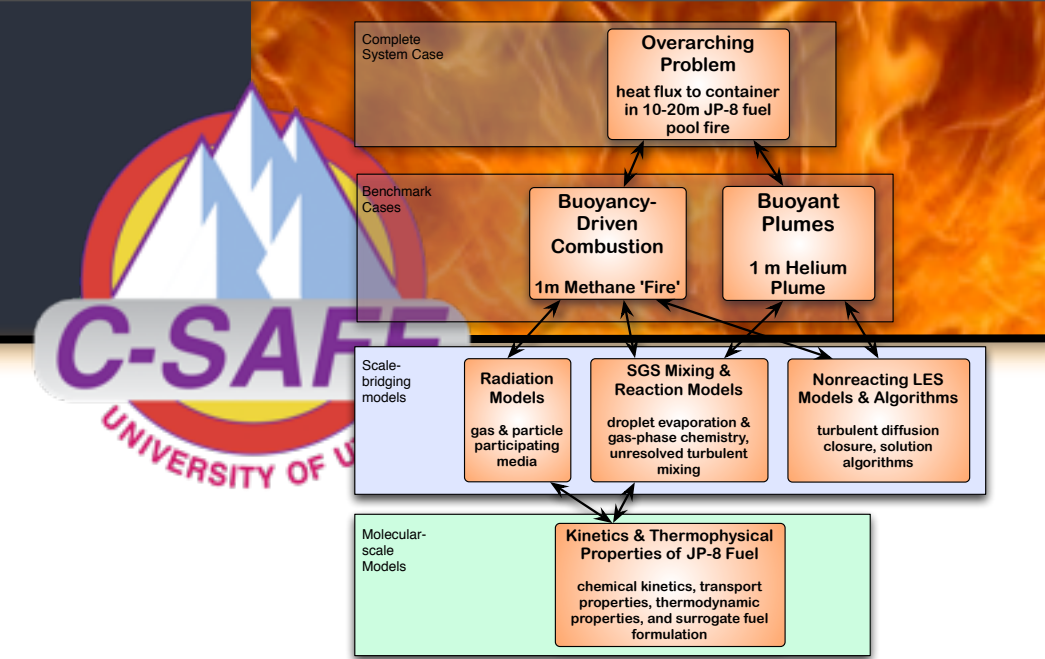
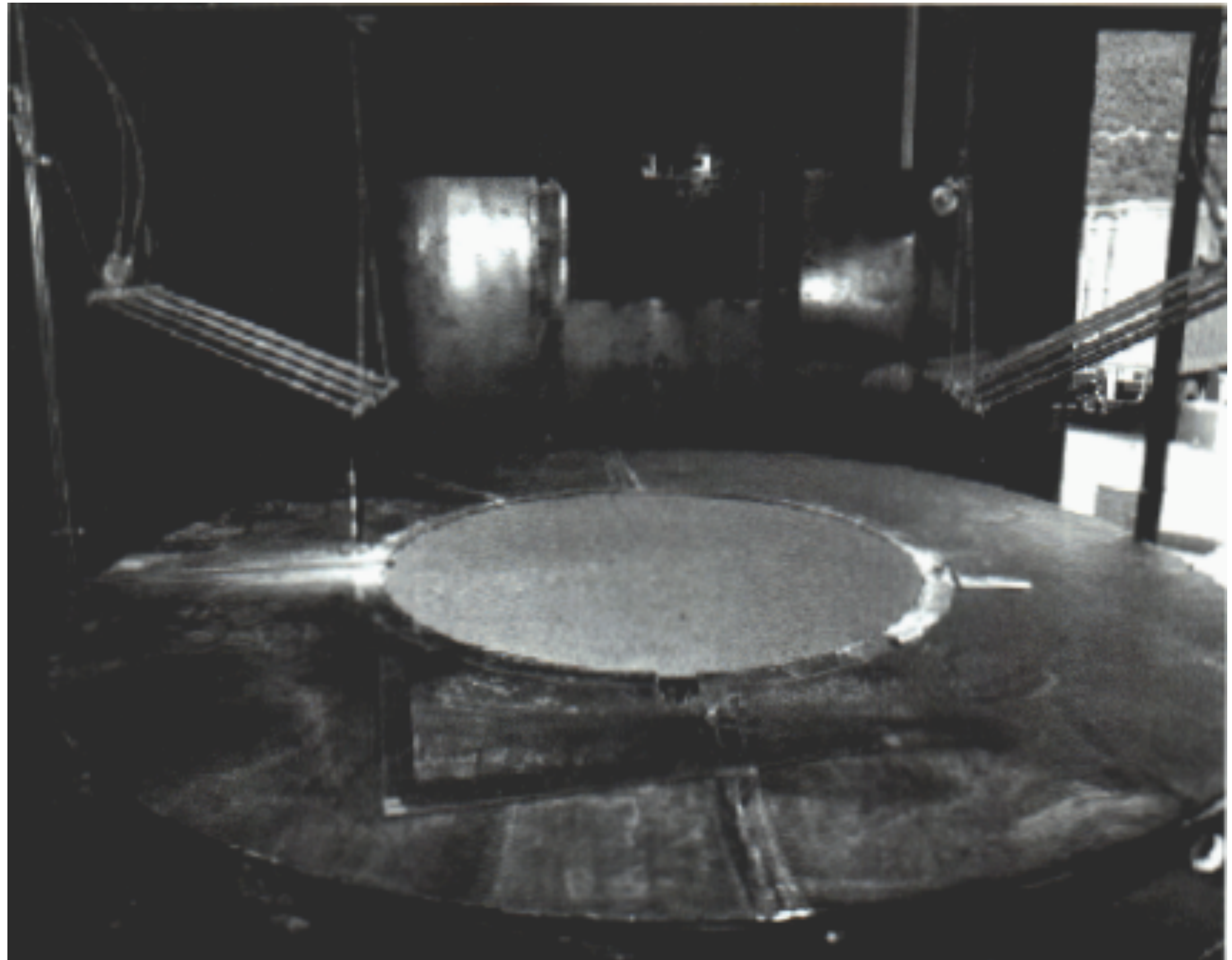
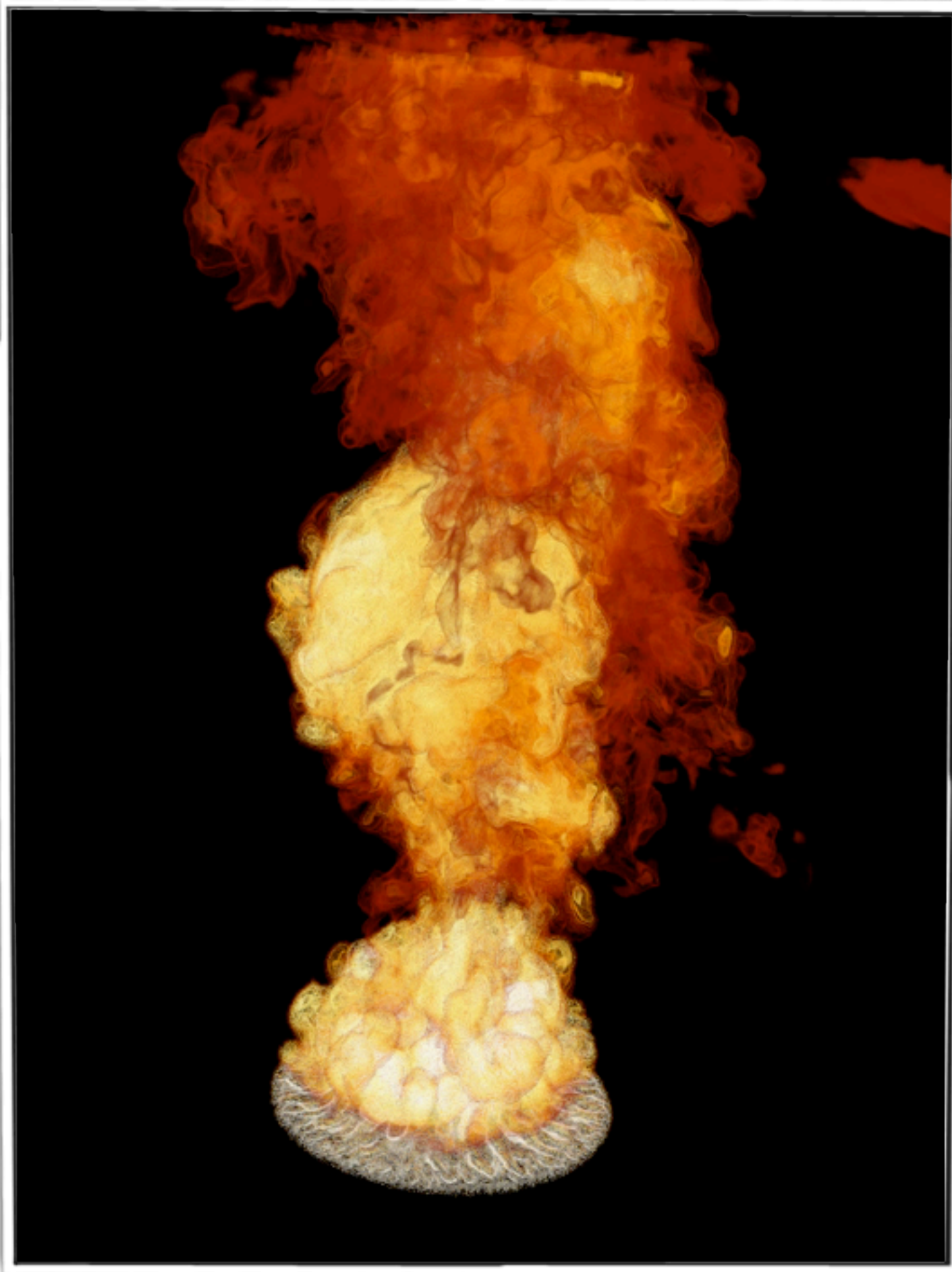
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Buoyant Plumes

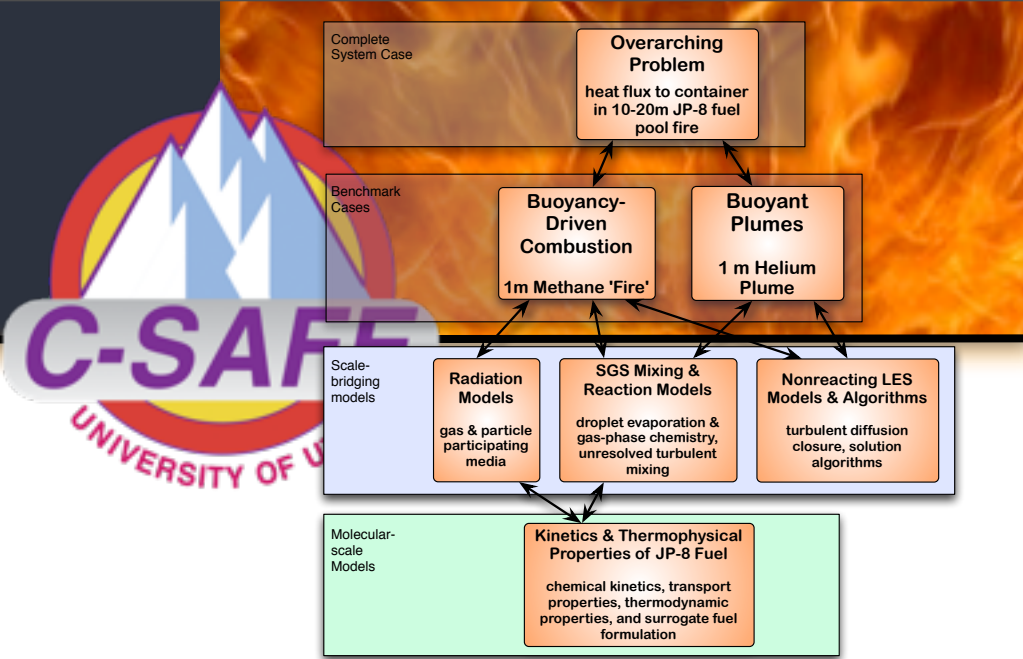
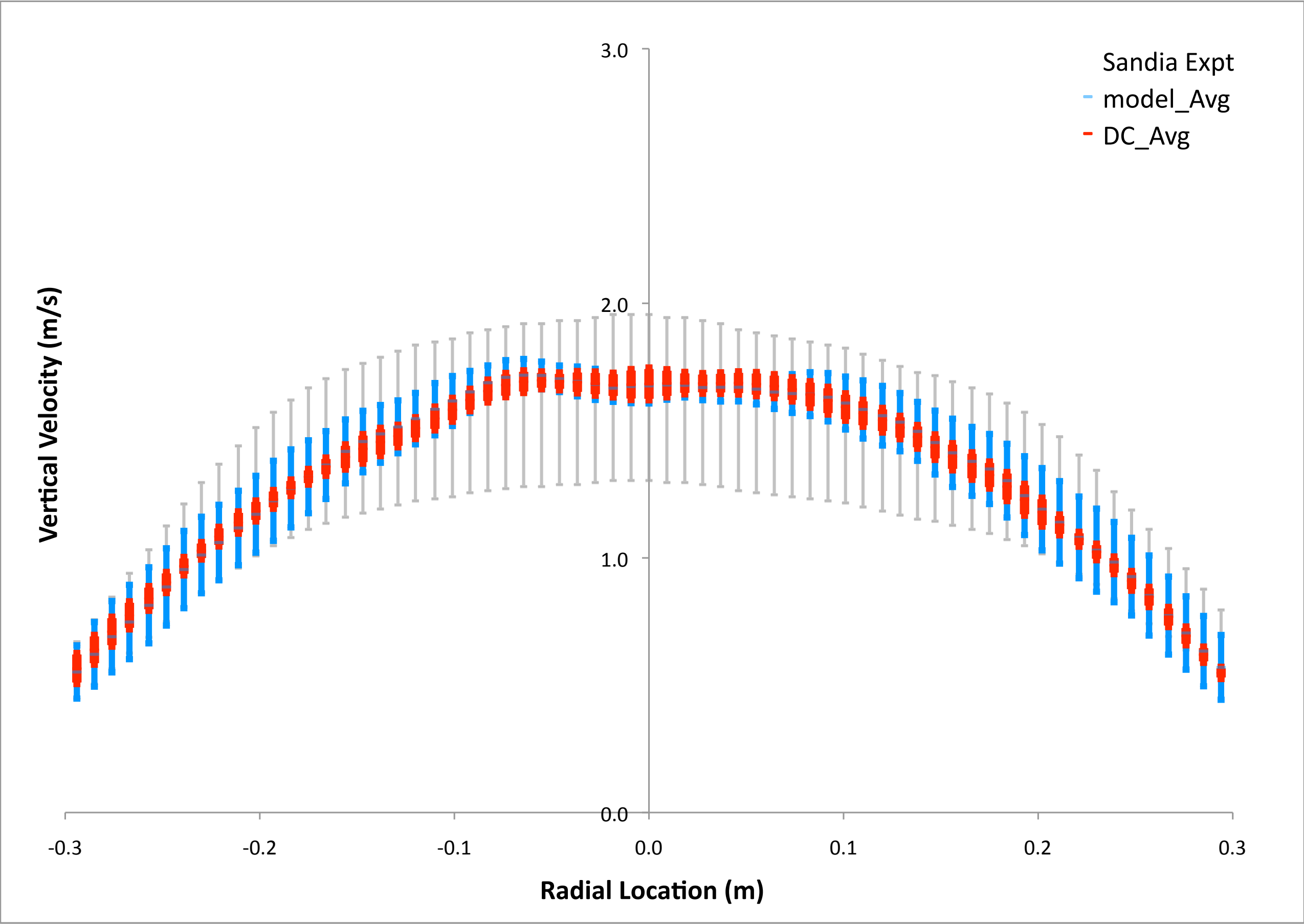
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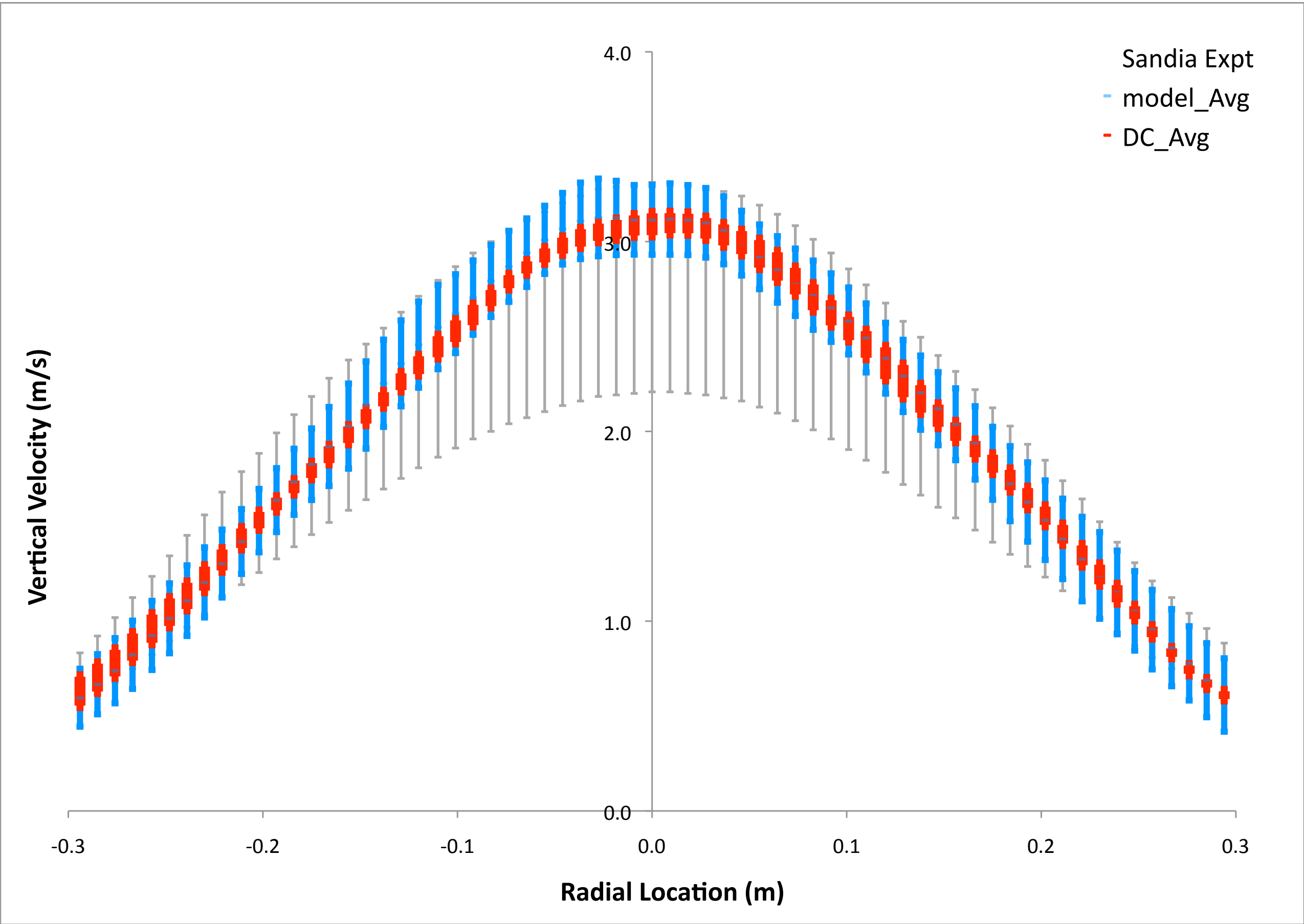
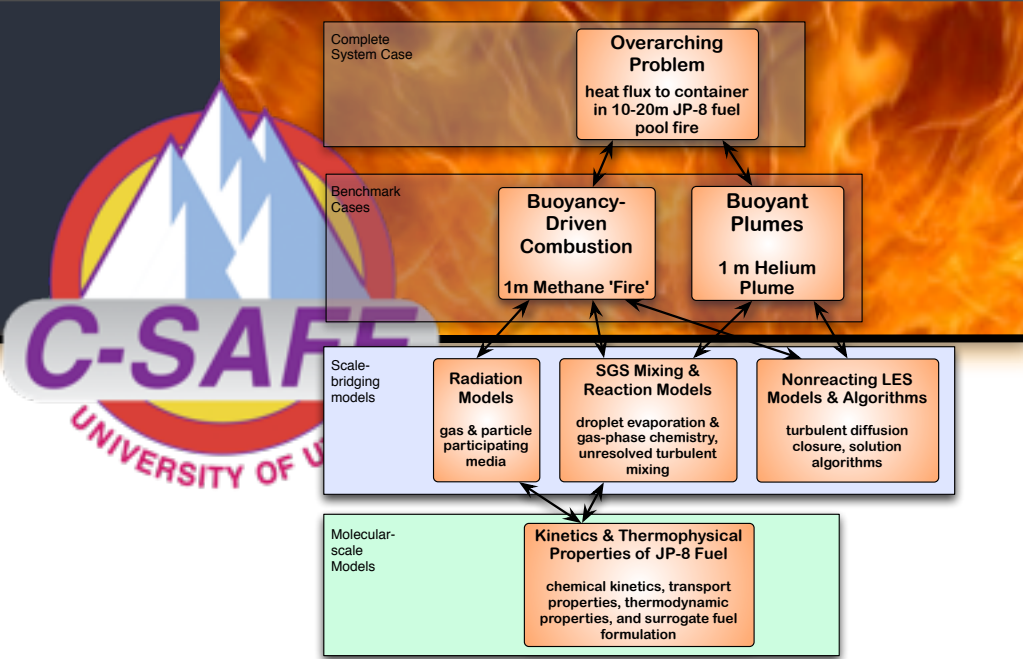
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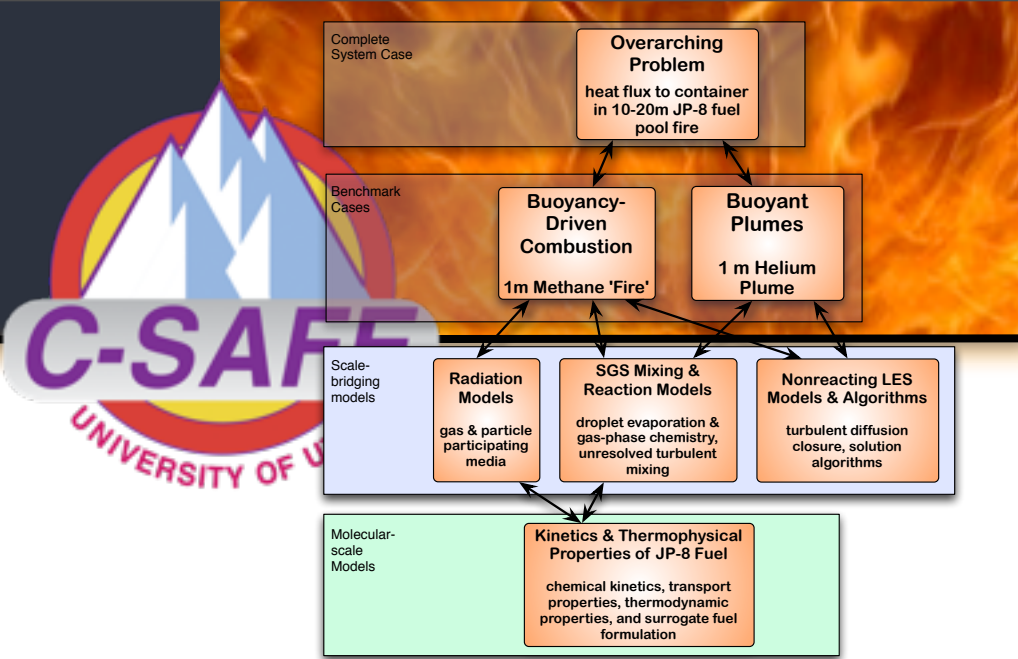
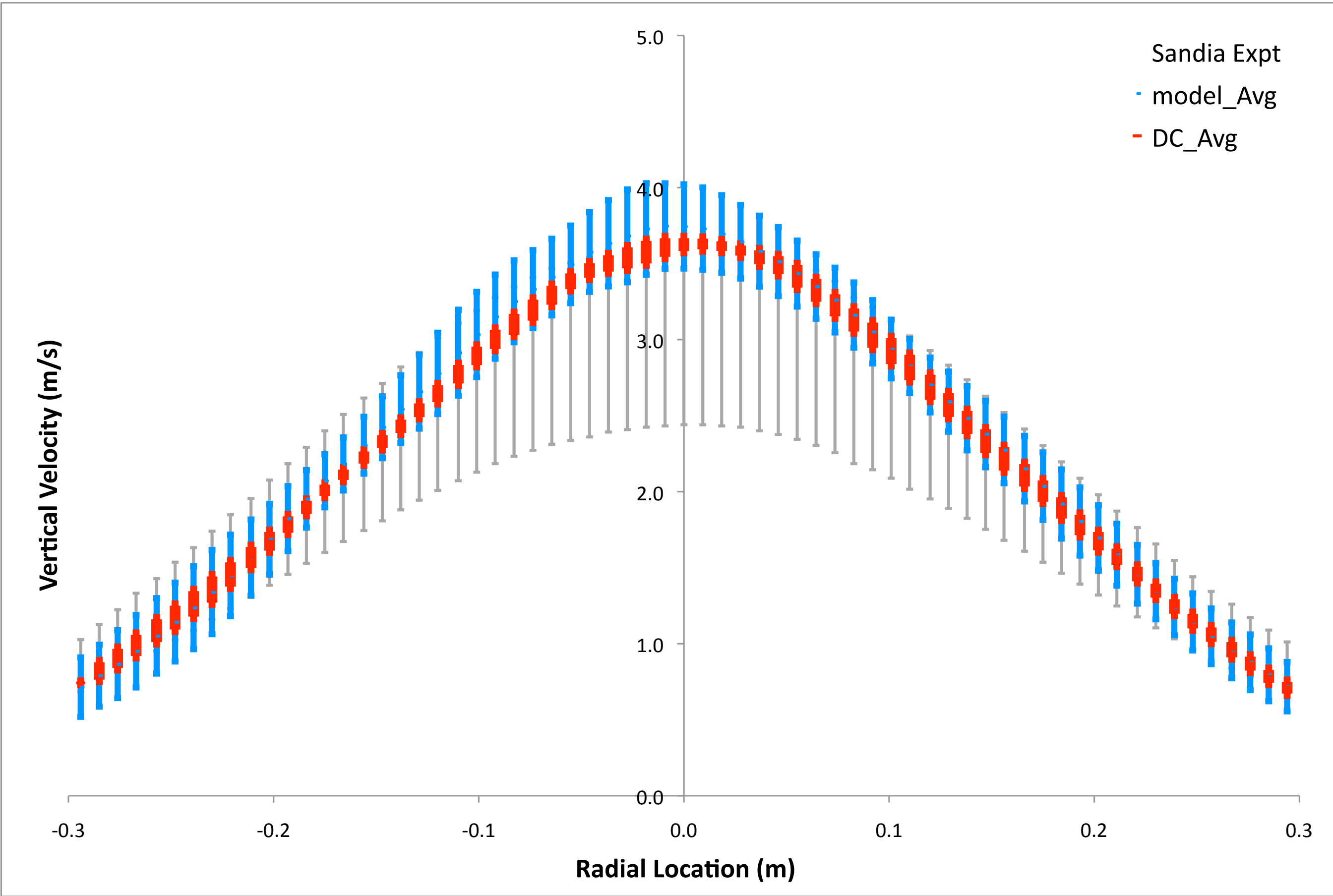
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Buoyant Plumes

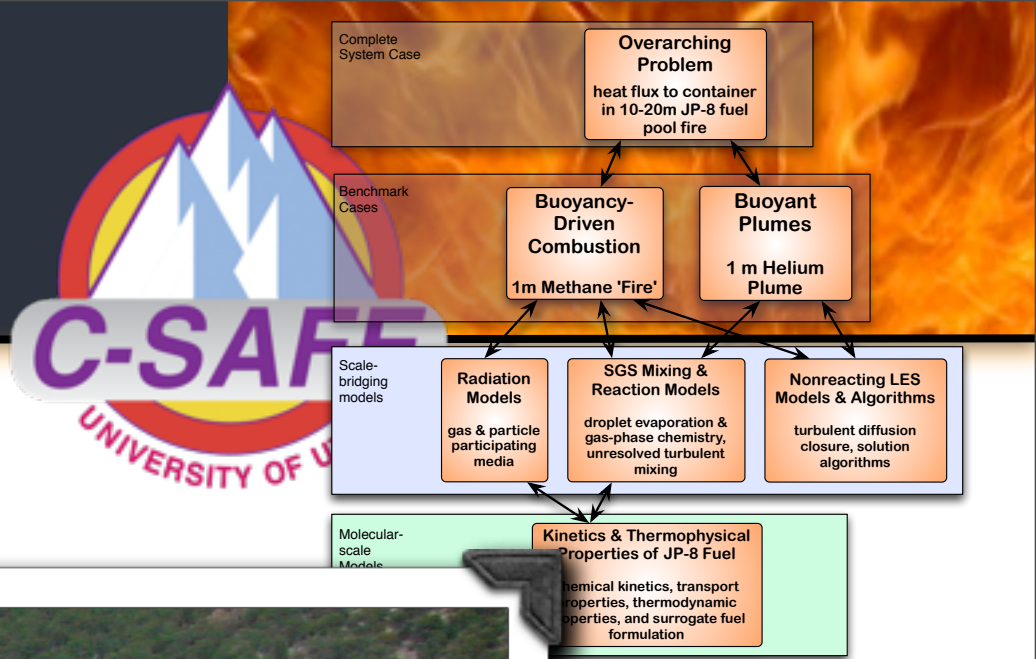
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experiments from Sandia FLAME facility - Tieszen et al. (Sandia National Laboratory)

Heat Flux from Large Pool Fires

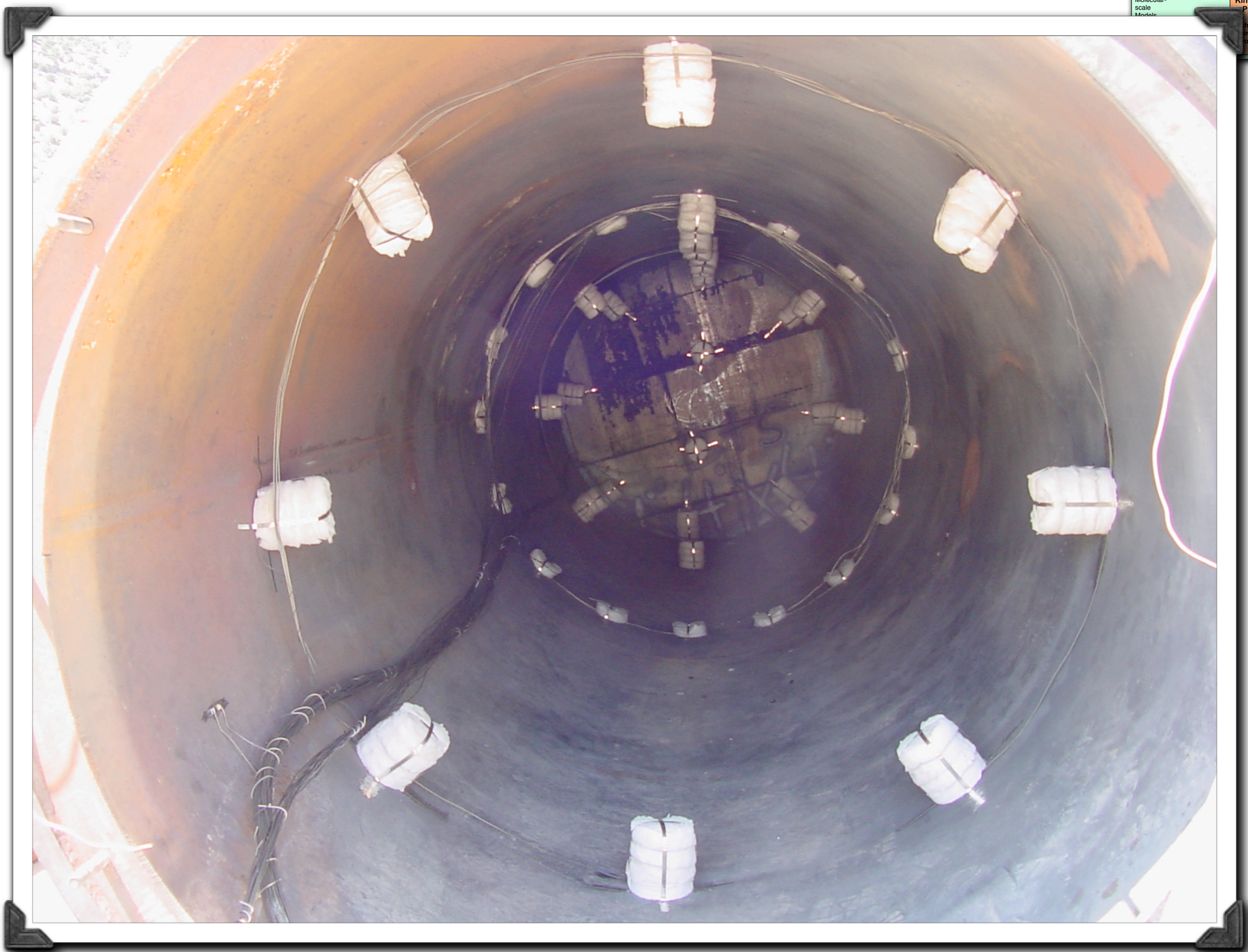
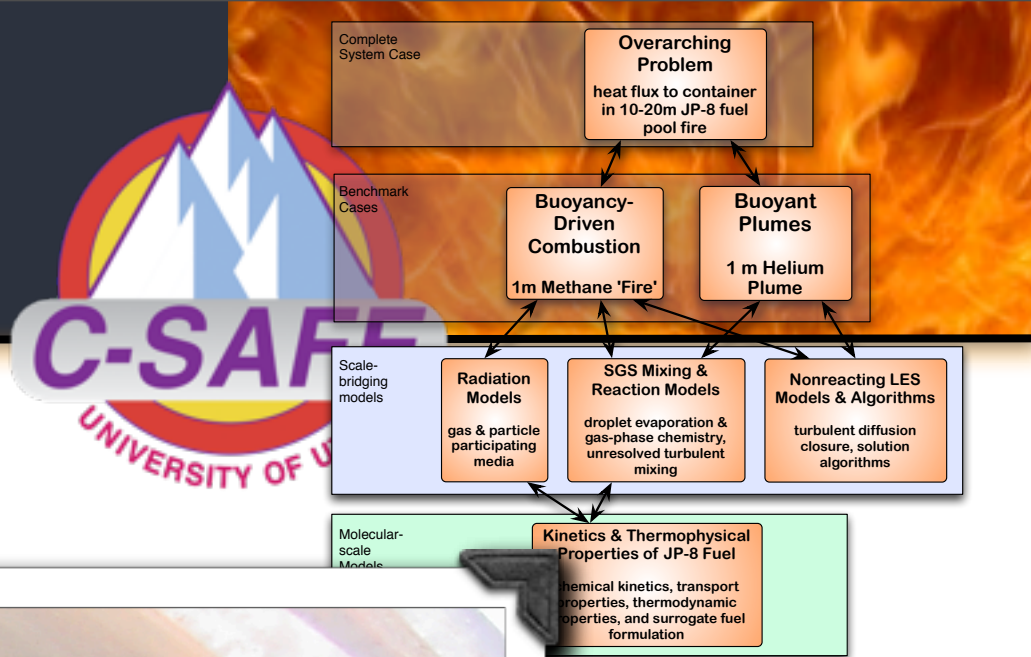
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experiments from Blanchat, Nicolette, Sundberg, Figueroa (SAND2006-7508)

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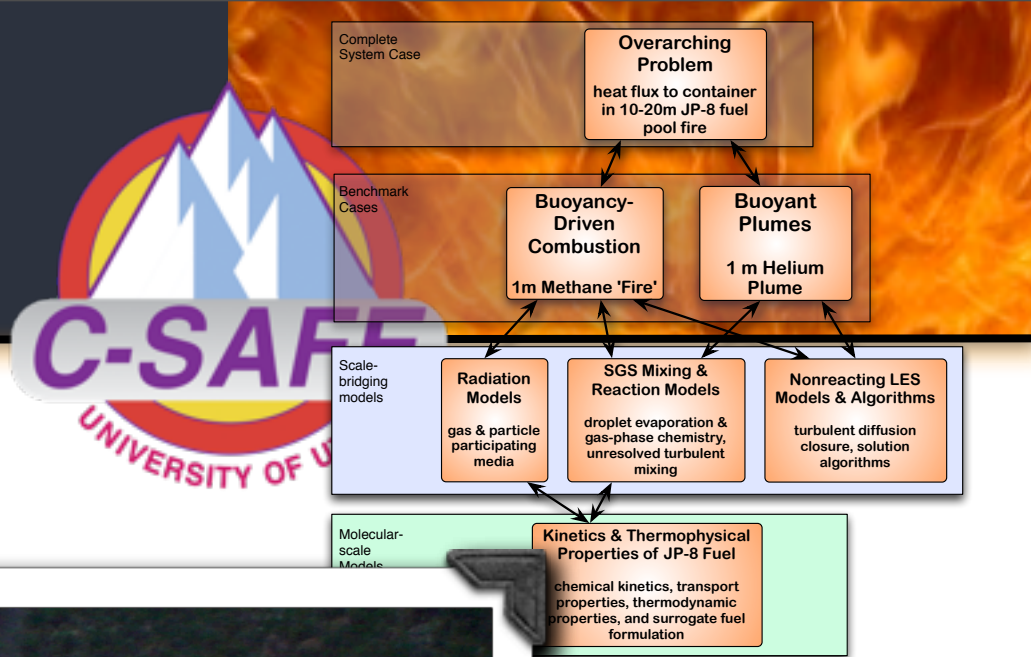
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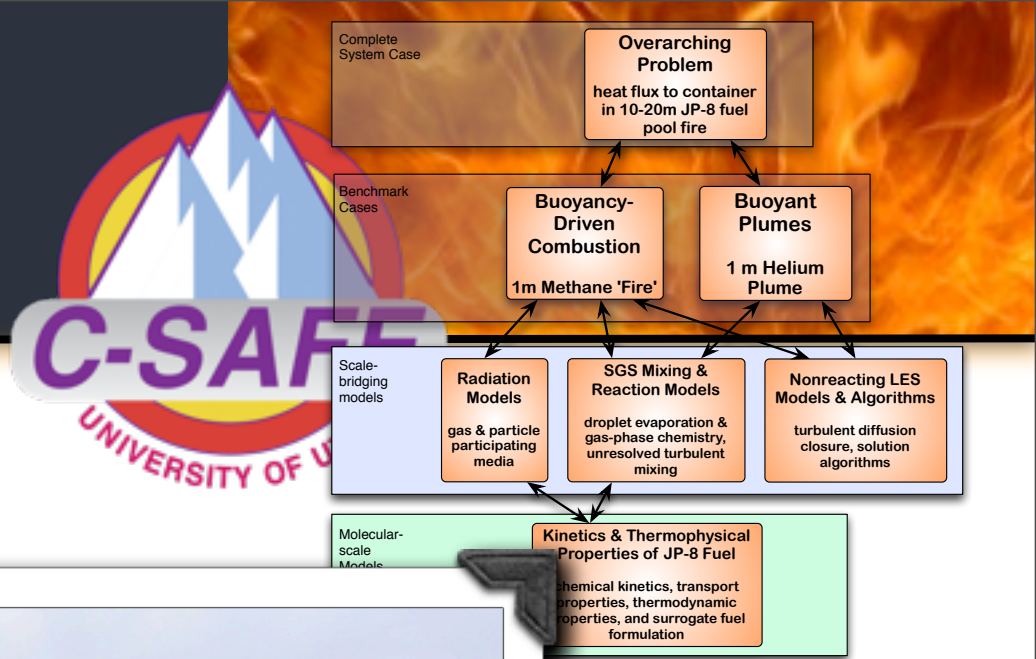
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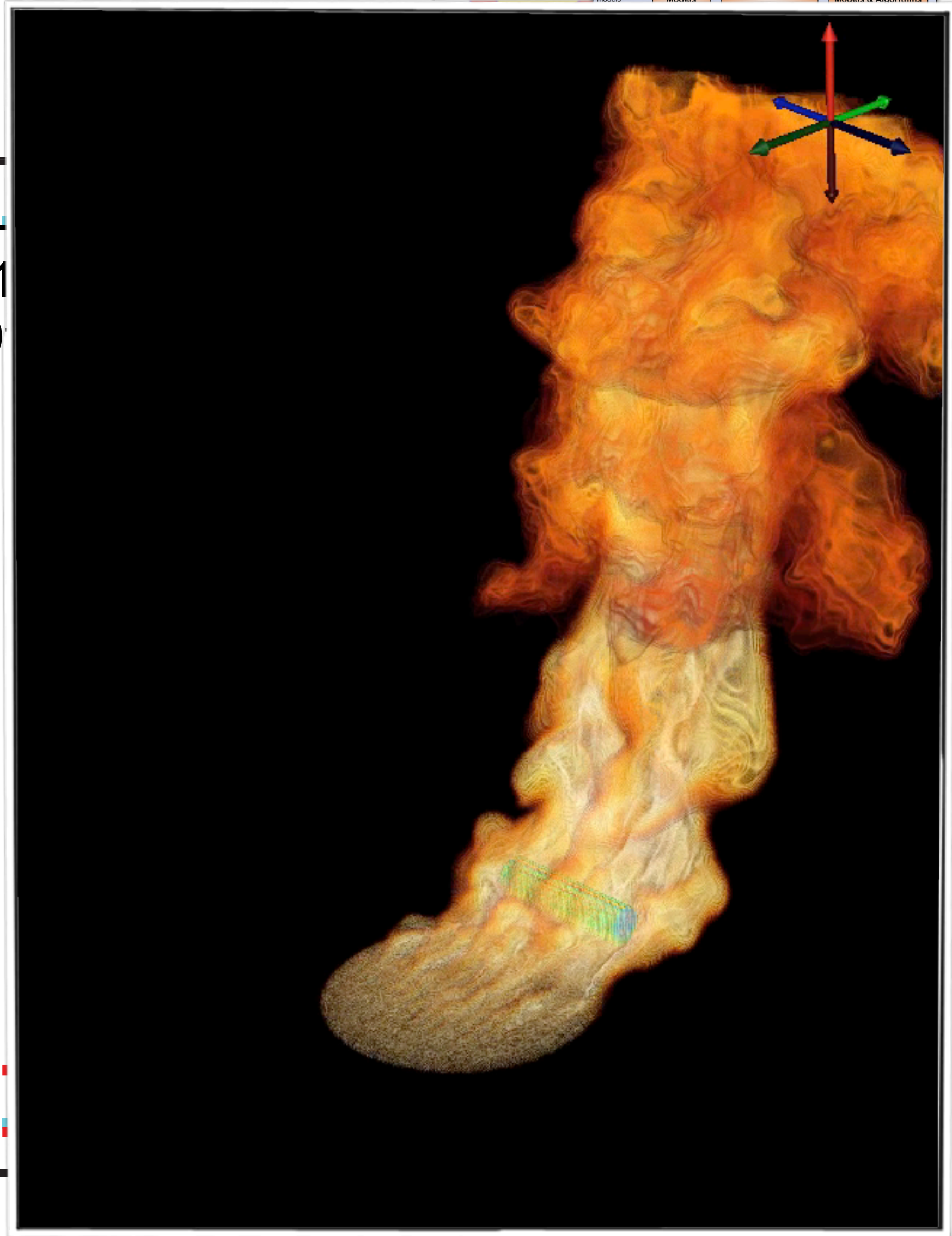
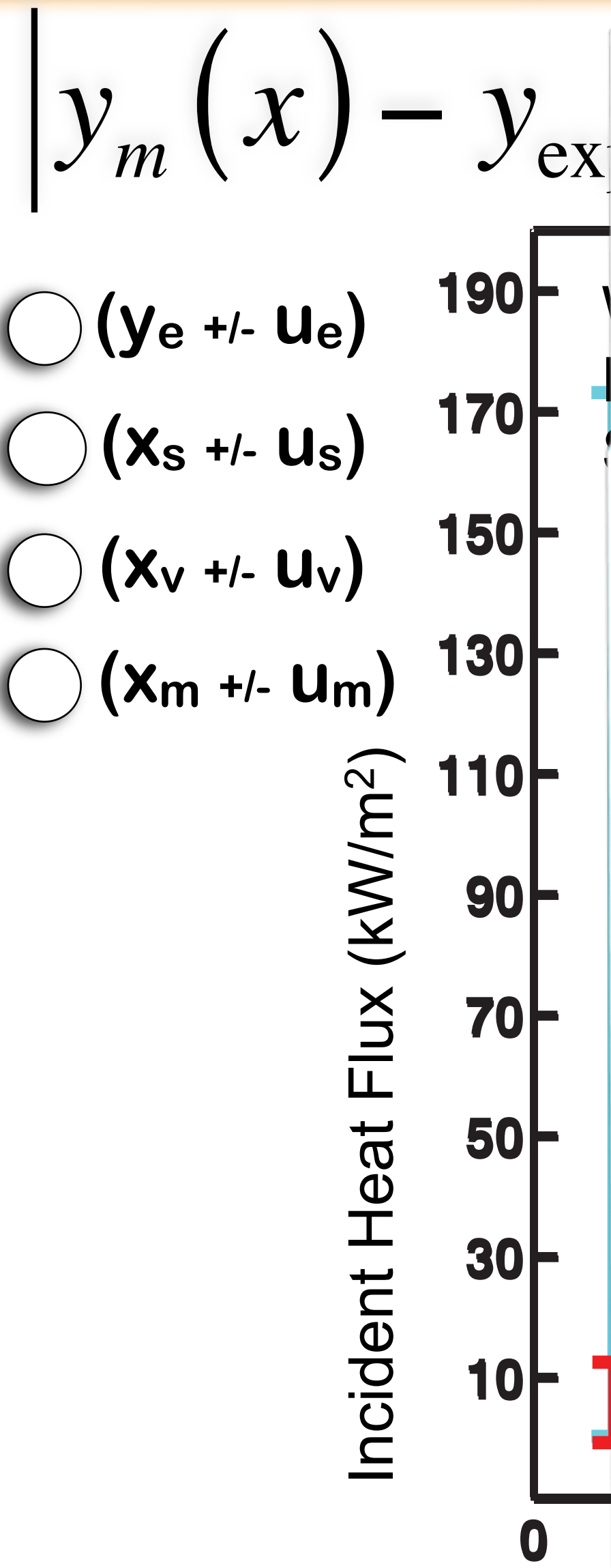
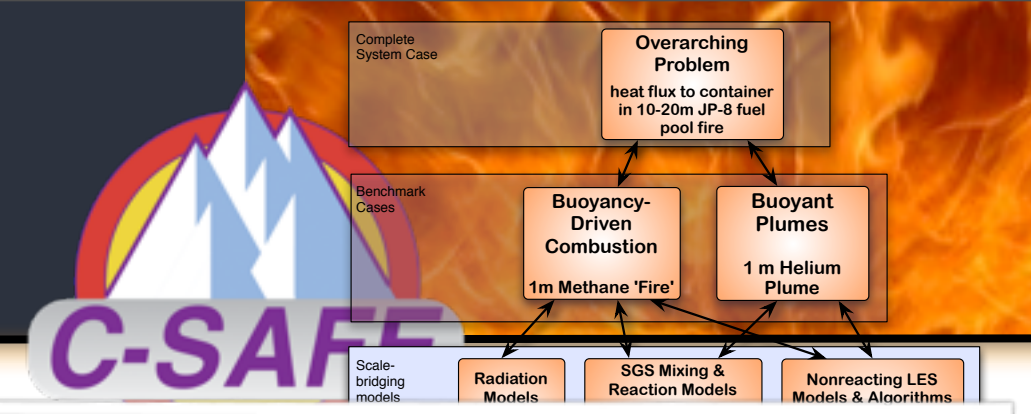
Heat Flux from Large Pool Fires

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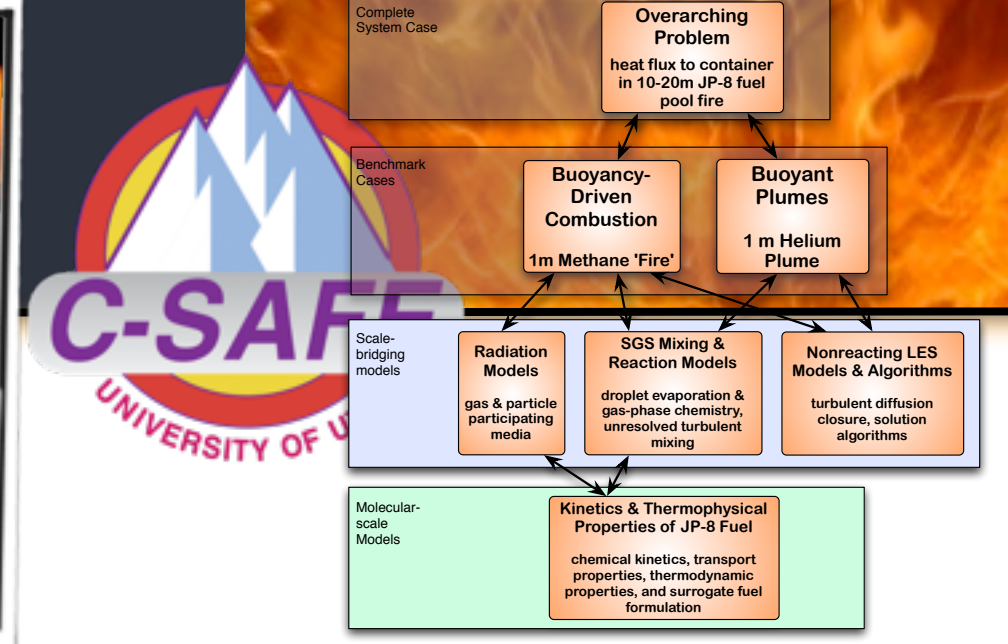
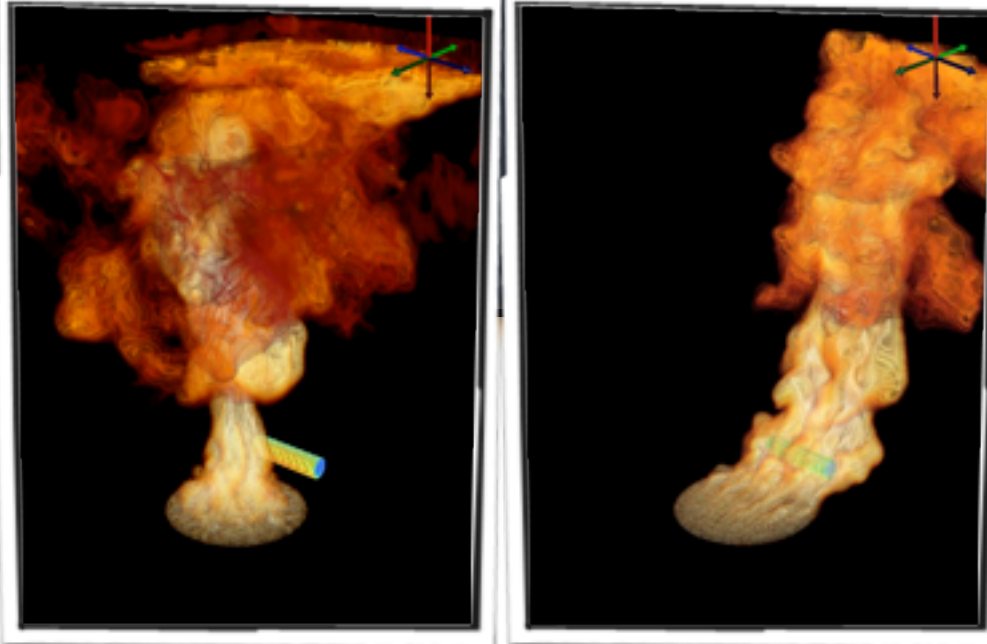
Heat Flux from Large Pool Fires



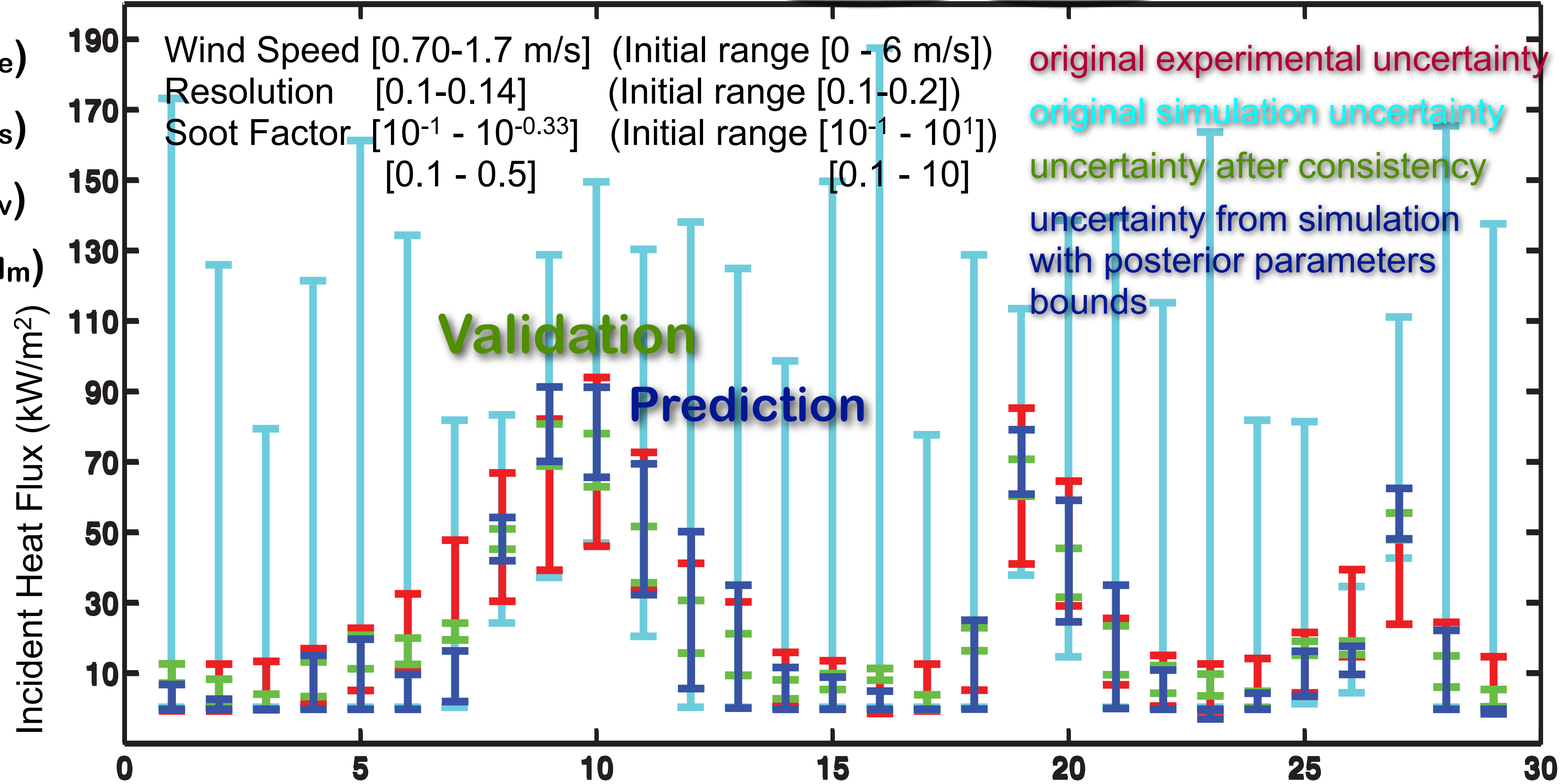
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Heat Flux from Large Pool Fires

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- $(y_e \pm u_e)$
- $(x_s \pm u_s)$
- $(x_v \pm u_v)$
- $(x_m \pm u_m)$



experiments from Blanchat, Nicolette, Sundberg, Figueroa (SAND2006-7508)

Sim. & Exp. - V/UQ: cost requirements



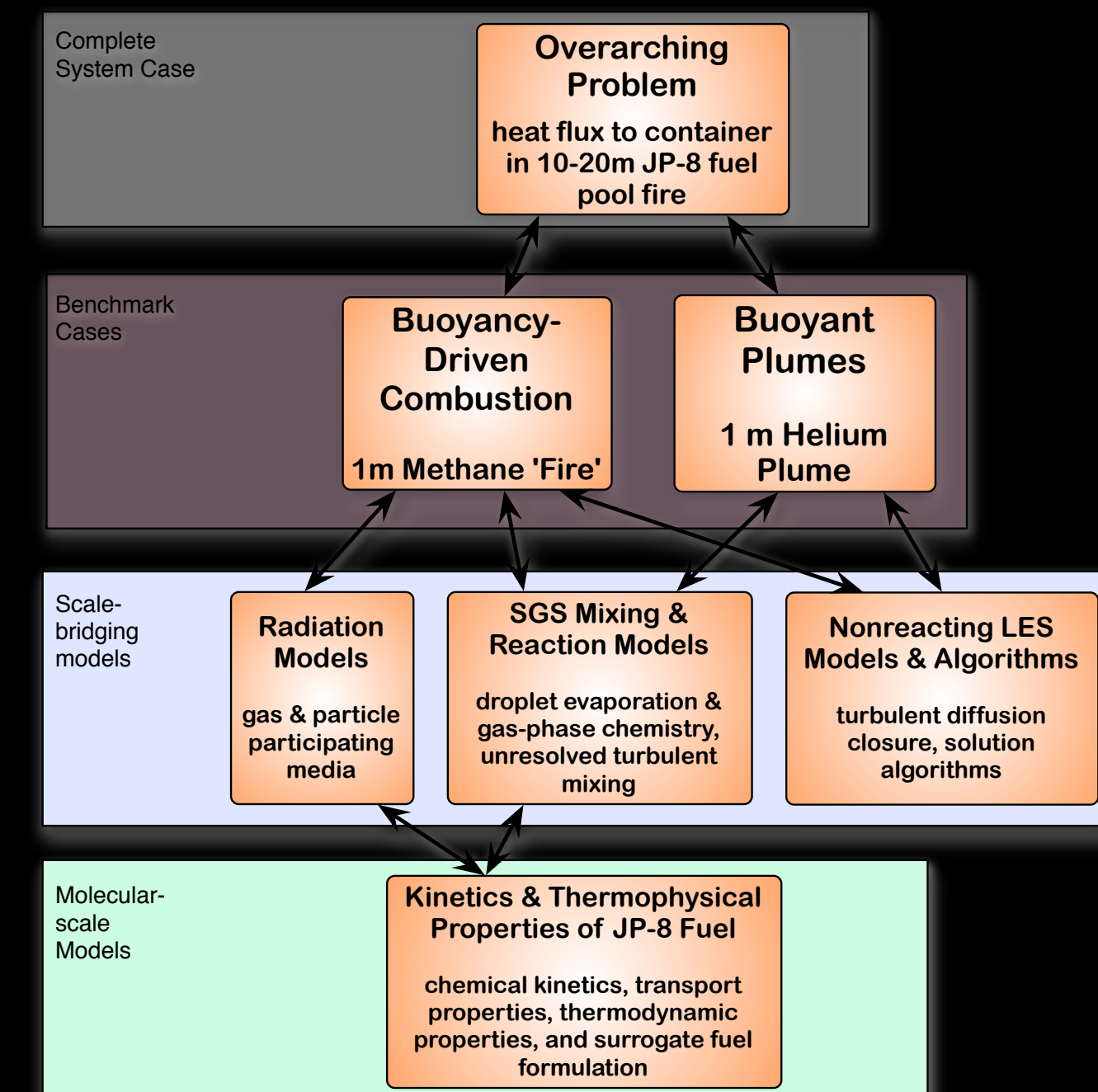
1. “All scientifically relevant data have an uncertainty.”
2. “Data without uncertainty cannot be relevant scientifically”

Manfred Drosig

- often expensive experiments & expensive simulations
- many more experiments are needed to quantify uncertainty
- many more simulations are needed to propagate error
- building a V/UQ computational framework

Predictivity (Error Budget)

- = $y(\text{numer. error, expt. error, model error, scenario error})$
- = lots of computing & lots of experiments



Sim. & Exp. - V/UQ: cost requirements

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